Connecting via Winsock to STN

```
Welcome to STN International! Enter x:x
```

LOGINID:ssspta1201txs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
      2
                 New pricing for the Save Answers for SciFinder Wizard within
NEWS
     3
         SEP 01
                 STN Express with Discover!
         OCT 28 KOREAPAT now available on STN
NEWS
         NOV 30 PHAR reloaded with additional data
NEWS
     5
        DEC 01 LISA now available on STN
NEWS
         DEC 09
     7
                12 databases to be removed from STN on December 31, 2004
NEWS
NEWS 8
        DEC 15
                 MEDLINE update schedule for December 2004
NEWS 9 DEC 17
                 ELCOM reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
     10 DEC 17
                 COMPUAB reloaded; updating to resume; current-awareness
NEWS
                 alerts (SDIs) affected
                 SOLIDSTATE reloaded; updating to resume; current-awareness
NEWS
      11 DEC 17
                 alerts (SDIs) affected
NEWS
      12 DEC 17
                 CERAB reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
NEWS
      13 DEC 17
                 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS
      14 DEC 30
                 EPFULL: New patent full text database to be available on STN
      15 DEC 30
NEWS
                 CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03
                 No connect-hour charges in EPFULL during January and
                 February 2005
NEWS
      17 JAN 26
                 CA/CAPLUS - Expanded patent coverage to include the Russian
                 Agency for Patents and Trademarks (ROSPATENT)
NEWS
     18 FEB 10
                STN Patent Forums to be held in March 2005
NEWS EXPRESS
              JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
NEWS WWW
              CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 12:26:22 ON 14 FEB 2005

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:26:30 ON 14 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2005 HIGHEST RN 830317-64-1 DICTIONARY FILE UPDATES: 13 FEB 2005 HIGHEST RN 830317-64-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

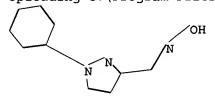
Please note that search-term pricing does apply when conducting SmartSELECT searches.

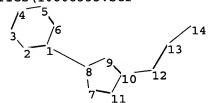
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10608333.str





chain nodes :

12 13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-8 10-12 12-13 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

1-8 7-8 8-9 9-10 12-13 13-14

exact bonds :

7-11 10-11 10-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 12:26:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 257 TO 903 PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> d scan

L2 5 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]N-hydroxy-5-[(hydroxyimino)methyl]-4-[(trifluoromethyl)thio]- (9CI)

MF C13 H7 Cl2 F6 N5 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 5 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-

(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI)

MF C12 H7 C12 F6 N5 O S

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 5 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

MF C14 H11 Cl2 F6 N5 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 ful

FULL SEARCH INITIATED 12:27:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 498 TO ITERATE

100.0% PROCESSED 498 ITERATIONS 91 ANSWERS

SEARCH TIME: 00.00.01

L3 91 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 161.76 161.97

FILE 'CAPLUS' ENTERED AT 12:27:33 ON 14 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 14 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 13 Feb 2005 (20050213/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

25 L3 L4

=> d l4 ibib hitstr abs 1-25

ANSWER 1 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:756697 CAPLUS

DOCUMENT NUMBER: 141:260772

TITLE: Preparation of N-arylheteroaryls, in particular

N-phenylpiperazinyl methanones, as inhibitors of tubulin polymerization and their compositions for

treatment of cancer

Le-Brun, Alain; Thompson, Fabienne; Tiraboschi, INVENTOR(S):

Gilles; Mailliet, Patrick; Salvino, Joseph M.

Aventis Pharma S.A., Fr. PATENT ASSIGNEE(S): PCT Int. Appl., 197 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIND				APPLICATION NO.									
													<del>-</del>					
WO	WO 2004078732			A1		20040916			WO 2004-FR168					20040126				
WO	O 2004078732			В1		2004	1028											
	W:	ΑE,	ΑE,	AG,	AL,	AL,	AM,	AM,	AM,	AT,	ΑT,	AU,	ΑZ,	ΑZ,	BA,	BB,	BG,	
		BG,	BR,	BR,	BW,	BY,	BY,	BZ,	BZ,	CA,	CH,	CN,	CN,	CO,	CO,	CR,	CR,	
		CU,	CU,	CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG,	ES,	
		ES,	FI,	FI,	GB,	GD,	GE,	GE,	GH,	GM,	HR,	HR,	HU,	HU,	ID,	IL,	IN,	
		IS,	JP,	JP,	KE,	ΚE,	KG,	KG,	KP,	KP,	ΚP,	KR,	KR,	KZ,	KZ,	ΚZ,	LC,	
		LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,	MW,	MX,	MX,	
		MZ,	MZ,	NA,	NI													
	RW:	BW,	GH,	GM,	KE,	LS;	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AT,	BE,	
		BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	LU,	
		MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	
		GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	
		GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG									
FR	FR 2850379				A1		2004	0730		FR 2	003-	894			2	0030	128	
PRIORITY APPLN. INFO.:			. :						FR 2	003-	894			A 2	0030	128		
										FR 2	003-	1308	6		A 2	0031	107	
OTHER SOURCE(S):				MAR	PAT	141:	2607	72			•							

756752-75-7P, (5E)-5-[[4-(3,5-Dimethoxyphenyl)piperazin-1yl]carbonyl]-1-phenyl-1H-pyrazole-3-carboxaldehyde oxime 756752-76-8P, (5Z)-5-[[4-(3,5-Dimethoxyphenyl)piperazin-1-

yl]carbonyl]-1-phenyl-1H-pyrazole-3-carboxaldehyde oxime
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
 (inhibitor of tubulin polymerization; preparation of N-arylheteroaryls, in
 particular N-phenylpiperazinyl methanones, as inhibitors of tubulin
 polymerization and their compns. for treatment of cancer)
RN 756752-75-7 CAPLUS
CN Piperazine, 1-(3,5-dimethoxyphenyl)-4-[[3-[(E)-(hydroxyimino)methyl]-1 phenyl-1H-pyrazol-5-yl]carbonyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.

T756752-77-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
 (intermediate; preparation of N-arylheteroaryls, in particular
 N-phenylpiperazinyl methanones, as inhibitors of tubulin polymerization and
 their compns. for treatment of cancer)
RN 756752-77-9 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[(Z)-(hydroxyimino)methyl]-1-phenyl-,
 ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

GI

$$\mathbb{R}^{3}$$
 $\mathbb{R}^{4}$ 
 $\mathbb{R}^{2}$ 
 $\mathbb{R}^{2}$ 
 $\mathbb{R}^{1}$ 

AB Title compds. I [wherein R1, R2 = independently (un)substituted hetero/aryl; L = CH2 and derivs., C(:O), C(:S), C:NOH and derivs.; R2 = (C5-C7)cycloalkyl; R3 = independently H, OH and derivs., S(O)nH and derivs., NH2 and derivs., halo, cycloalkylene, (un)substituted hetero/aryl, cycloalkyl, alkyl, etc.; R4 = H, alk(en/yn)yl, cyclopropyl, alkoxy, S-alkyl, F, Cl, Br; n = 0-2; X = N, CH; G = substituted piperazine, piperidine, 1,2,5,6-tetrahydropyridine; their racemics, stereoisomers, tautomers, prodrugs, and pharmaceutical acceptable salts] were prepared as inhibitors of tubulin polymerization and of tumor and

were prepared as inhibitors of tubulin polymerization and of tumor and endothelial cell proliferation in vitro, and for use in treatment of cancer. A

combinatorial library of N-phenylpiperazinyl pyrazolyl ketones is given. For example, II was prepared from 5-methyl-2-phenyl-2H-pyrazole-3-carboxylic acid and 1-(3-chlorophenyl)piperazine. II gave an IC50 of 0.2  $\mu\text{M}$  for inhibition of tubulin polymerization, an IC50 value of 0.002  $\mu\text{M}$  for inhibition of HCT116 cells proliferation, and a 22% detachment of the endothelial HDMEC cells at a concentration of 1  $\mu\text{M}$ . Thus, I and their pharmaceutical

compns. are useful for treating cancer (no data).

REFERENCE COUNT: THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:252948 CAPLUS

DOCUMENT NUMBER: 140:423618

TITLE: Synthesis and Selective Cyclooxygenase-2 Inhibitory

Activity of a Series of Novel, Nitric Oxide

Donor-Containing Pyrazoles

Ranatunge, Ramani R.; Augustyniak, Michael; Bandarage, AUTHOR (S):

Upul K.; Earl, Richard A.; Ellis, James L.; Garvey, David S.; Janero, David R.; Letts, L. Gordon; Martino, Allison M.; Murty, Madhavi G.; Richardson, Stewart K.; Schroeder, Joseph D.; Shumway, Matthew J.; Tam, S.

William; Trocha, A. Mark; Young, Delano V.

NitroMed Inc., Bedford, MA, 01730, USA CORPORATE SOURCE:

SOURCE: Journal of Medicinal Chemistry (2004), 47(9),

2180-2193

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal English LANGUAGE:

TΨ 640727-97-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(preparation and selective cyclooxygenase-2 inhibitory activity of nitric

oxide donor-containing pyrazoles)

640727-97-5 CAPLUS RN

CNBenzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

Me

 $O_2N - O - (CH_2)_3$ HO-

GI

AB The synthesis of a series of novel pyrazoles containing a nitrate (ONO2) moiety as a nitric oxide (NO)-donor functionality is reported. Their COX-1 and COX-2 inhibitory activities in human whole blood are profiled. The data demonstrate that pyrazole ring substituents play an important role in COX-2 selective inhibition, such that a cycloalkylpyrazole (I, X = CH2) was found to be a potent and selective COX-2 inhibitor. Other modifications at the 3 position of the central pyrazole ring [I, X =(CH2)3, C(:NOH)(CH2)3, (Z)-CH:CHCH2CH2] enhanced COX-2 inhibitory potency. Among the pyrazoles synthesized, the oxime [I, X = C(:NOH)(CH2)3] was identified as the most potent COX-2 selective inhibitor. Accordingly, this compound was profiled pharmacol. in the rat after oral administration and shown to possess potent antiinflammatory activity in the carrageenan-induced air-pouch model and less gastric toxicity than a standard COX-2 inhibitor when administered with background aspirin treatment. The enhanced gastric tolerance of an NO-donor COX-2 selective inhibitor has the potential to augment the clin. profile of this drug class.

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

Ι

ACCESSION NUMBER: 2004:20441 CAPLUS

DOCUMENT NUMBER: 140:77147

TITLE: Preparation of optionally nitrosated and/or

nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compositions and methods of use

INVENTOR(S): Garvey, David S.; Ranatunge, Ramani R.; Richardson,

Stewart K.

PATENT ASSIGNEE(S): Nitromed, Inc., USA

SOURCE: PCT Int. Appl., 166 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.			KIND DATE				APPLICATION NO.					DATE					
				-													
WO 2004002420			A2	A2 20040108				WO 2003-US20421					20030630				
WO 2004002420			<b>A3</b>	A3 20040701													
1	<b>W</b> :	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	ŪĠ,	US,	UΖ,	VC,	VN,	YŪ,	ZA,	ZM,	ZW						
;	RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,

KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG PRIORITY APPLN. INFO:

US 2002-392044P P 20020628

OTHER SOURCE(S):

MARPAT 140:77147

IT 640727-83-9P, 1-[3-[1-(Hydroxyimino)-4-(nitrooxy)butyl]-1phenylpyrazol-5-yl]-4-(methylsulfonyl)benzene 640727-97-5P,
4-[3-[1-(Hydroxyimino)-4-(nitrooxy)butyl]-5-[4(methylsulfonyl)phenyl]pyrazol-1-yl]benzenecarbonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of optionally nitrosated and/or nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compns. and methods of use)

RN 640727-83-9 CAPLUS

CN 1-Butanone, 1-[5-[4-(methylsulfonyl)phenyl]-1-phenyl-1H-pyrazol-3-yl]-4-(nitrooxy)-, oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & \\ & & \\$$

RN 640727-97-5 CAPLUS
CN Benzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

$$O_2N-O-(CH_2)_3-C$$
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 

GI

$$\begin{array}{c}
 & (R^1)_{1?4} \\
 & c \\
 & z^1 \\
 & x^1
\end{array}$$

$$\begin{array}{c} & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

The invention describes novel cyclooxygenase 2 (COX-2) selective AB inhibitors having at least one oxime group or hydrazone group optionally nitrosated and/or nitrosylated (one class shown as I; variables defined below; e.g. II; 15 other classes of compds. are also described in the 1st claim) and novel compns. and kits comprising at least one I and optionally, at least one compound that donates, transfers or releases nitric oxide, stimulates endogenous synthesis of nitric oxide, elevates endogenous levels of endothelium-derived relaxing factor or is a substrate for nitric oxide synthase, and/or at least one therapeutic agent. The invention also provides methods for treating inflammation, pain and fever; for treating and/or improving the gastrointestinal properties of COX-2 selective inhibitors; for facilitating wound healing; for treating and/or preventing renal and/or respiratory toxicity; for treating and/or preventing other disorders resulting from elevated levels of cyclooxygenase-2; and for improving the cardiovascular profile of COX-2 selective inhibitors. Six examples of I were tested for inhibition of COX-1 and COX-2; e.g. 1-[1-cyclohexyl-3-[1-(hydroxyimino)-4-(nitrooxy)butyl]pyrazol-4-yl]-4-(methylsulfonyl)benzene inhibited COX-1 10 % at 100  $\mu M$  and COX-2 100 % at 10  $\mu M$ . Although the methods of preparation are not claimed, 6 example prepns. are included. For example, II was prepared in 7 steps (79, 68, 84, 79, 51, 84 and 48 % yields, resp.) starting from di-Me oxalate, NaOMe and 4'-(methylthio)acetophenone in toluene and involving intermediates Me (2Z)-2-hydroxy-4-(4methylthiophenyl) -4-oxobut-2-enoate, Me 5-(4-methylthiophenyl) -1phenylpyrazole-3-carboxylate, N-methoxy-N-methyl-5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxamide, 1-[5-(4-methylthiophenyl)-1-phenylpyrazol-3yl]-4-(1,1,2,2-tetramethyl-1-silapropoxy)butan-1-one, 4-hydroxy-1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]butan-1-one, and 1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]-4-(nitrooxy)butan-1one. For I: when side b is a double bond, and sides a and c are single bonds, -X1-Y1-Z1- is: -CR4(R5)CR5(R5')CR4(R5)-, -C(0)CR4(R4')CR5(R5')-, -CR4(R4')CR5(R5')C(0)-, -[CR5(R5')]kOC(0)-, etc.; when sides a and c are double bonds and side b is a single bond, -X1-Y1-Z1- is: :CR4OCR5:,

II

:CR4NR3CR5:, :NSCR4:, :CR4SN:, etc. R1 is S(0)2Me, S(0)2NR8(D1), S(0) 2N(D1)C(0)CF3, S(0)(NH)NH(D1), S(0)(NH)N(D1)C(0)CF3, P(0)MeNH(D1), P(O)Me2, C(S)NH(D1), S(O)(NH)Me, P(O)MeOD1, or P(O)MeNH(D1); R1' is H, halo, Me, or CH2OH. R2 is lower alkyl, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, mono, di- or trisubstituted heteroaryl (wherein the heteroaryl is a monocyclic aromatic ring of 5 atoms, said ring having one heteroatom which is S, O, or N, and, optionally, 1-3 addnl. N atoms; or the heteroaryl is a monocyclic ring of 6 atoms, said ring having one heteroatom which is N, and, optionally, 1-4 addnl. N atoms), benzoheteroaryl, NR10R11, SR11, OR11, R11, alkenyl, alkynyl, unsubstituted, mono, di, tri- or tetrasubstituted cycloalkenyl, mono, di, tri- or tetrasubstituted heterocycloalkyl group of 5-7 members, or a benzoheterocycle, wherein said heterocycloalkyl or benzoheterocycle contains 1 or 2 heteroatoms selected from O, S, or N and, optionally, contains a carbonyl group or a sulfonyl group, styryl, mono or disubstituted styryl, phenylacetylene, mono- or disubstituted phenylacetylene, fluoroalkenyl, mono- or disubstituted bicyclic heteroaryl of 8-10 members, containing 2-5 heteroatoms (wherein at least one heteroatom resides on each ring of said bicyclic heteroaryl, said heteroatoms are each independently O, S and N), K, aryl, arylalkyl, cycloalkylalkyl, -C(O)R11, hydrogen, arylalkenyl, arylalkoxy, alkoxy, aryloxy, cycloalkoxy, arylthio, alkylthio, arylalkylthio, or cycloalkylthio. R3 is hydrogen, haloalkyl (preferably CF3), CN, lower alkyl, [C(Re)(Rf)]p-U-V, K, (un) substituted lower alkyl-Q, lower alkyl-O-lower alkyl-Q, etc., Q, alkylcarbonyl, arylcarbonyl, alkylarylcarbonyl, arylalkylcarbonyl, carboxylic ester, carboxamido, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, alkenyl, alkynyl, arylalkyl, lower alkyl-OD1, alkoxyalkyl, aminoalkyl, lower alkyl-CO2R10, lower alkyl-C(O)NR10(R10'), heterocyclic alkyl, or heterocyclic ring-C(0)-; with the proviso that one oxime or hydrazone group must be present; addnl. details are given in the claims.

```
ANSWER 4 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
```

ACCESSION NUMBER:

2004:20345 CAPLUS

DOCUMENT NUMBER: TITLE:

140:77144 Preparation of optionally nitrosated and/or

nitrosylated oxime and/or hydrazone cyclooxygenase-2

INVENTOR(S):

selective inhibitors, compositions and methods of use Ranatunge, Ramani R.; Garvey, David S.; Richardson,

Stewart K.

PATENT ASSIGNEE(S):

Nitromed, Inc., USA

SOURCE:

U.S. Pat. Appl. Publ., 74 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPL]	DATE		
					· <b>-</b>	
US 2004006133	A1	20040108	US 20	003-608333		20030630
PRIORITY APPLN. INFO.:			US 20	002-392044P	P	20020628
OTHER SOURCE(S):	MARPAT	140:77144				

640727-83-9P 640727-97-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of optionally nitrosated and/or nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compns. and methods of use)

640727-83-9 CAPLUS RN

CN 1-Butanone, 1-[5-[4-(methylsulfonyl)phenyl]-1-phenyl-1H-pyrazol-3-yl]-4-(nitrooxy)-, oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & \\ & & \\$$

RN 640727-97-5 CAPLUS
CN Benzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

$$O_2N-O-(CH_2)_3-C$$
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 

GI

AB The invention describes novel cyclooxygenase 2 (COX-2) selective inhibitors having at least one oxime group or hydrazone group optionally nitrosated and/or nitrosylated (one class shown as I; variables defined below; e.g. II; 15 other classes of compds. are also described in the 1st claim) and novel compns. and kits comprising at least one I and optionally, at least one compound that donates, transfers or releases nitric oxide, stimulates endogenous synthesis of nitric oxide, elevates endogenous levels of endothelium-derived relaxing factor or is a substrate for nitric oxide synthase, and/or at least one therapeutic agent. The invention also provides methods for treating inflammation, pain and fever; for treating and/or improving the gastrointestinal properties of COX-2 selective inhibitors; for facilitating wound healing; for treating and/or preventing renal and/or respiratory toxicity; for treating and/or preventing other disorders resulting from elevated levels of cyclooxygenase-2; and for improving the cardiovascular profile of COX-2 selective inhibitors. Six examples of I were tested for inhibition of COX-1 and COX-2; e.g. 1-[1-cyclohexyl-3-[1-(hydroxyimino)-4-(nitrooxy)butyl]pyrazol-4-yl]-4-(methylsulfonyl)benzene inhibited COX-1 10 % at 100  $\mu M$  and COX-2 100 % at 10  $\mu M$ . Although the methods of preparation are not claimed, 6 example prepns. are included. For example, II was prepared in 7 steps (79, 68, 84, 79, 51, 84 and 48 % yields, resp.) starting from di-Me oxalate, NaOMe and 4'-(methylthio)acetophenone in toluene and involving intermediates Me (2Z)-2-hydroxy-4-(4methylthiophenyl)-4-oxobut-2-enoate, Me 5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxylate, N-methoxy-N-methyl-5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxamide, 1-[5-(4-methylthiophenyl)-1-phenylpyrazol-3yl]-4-(1,1,2,2-tetramethyl-1-silapropoxy)butan-1-one, 4-hydroxy-1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]butan-1-one, and 1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]-4-(nitrooxy)butan-1one. For I: when side b is a double bond, and sides a and c are single bonds, -X1-Y1-Z1- is: -CR4(R5)CR5(R5')CR4(R5)-, -C(0)CR4(R4')CR5(R5')-, -CR4(R4')CR5(R5')C(0)-, -[CR5(R5')]kOC(0)-, etc.; when sides a and c are double bonds and side b is a single bond, -X1-Y1-Z1- is: :CR40CR5:,

II

:CR4NR3CR5:, :NSCR4:, :CR4SN:, etc. R1 is S(0)2Me, S(0)2NR8(D1), S(0) 2N(D1)C(0)CF3, S(0)(NH)NH(D1), S(0)(NH)N(D1)C(0)CF3, P(0)MeNH(D1), P(O)Me2, C(S)NH(D1), S(O)(NH)Me, P(O)MeOD1, or P(O)MeNH(D1); R1' is H, halo, Me, or CH2OH. R2 is lower alkyl, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, mono, di- or trisubstituted heteroaryl (wherein the heteroaryl is a monocyclic aromatic ring of 5 atoms, said ring having one heteroatom which is S, O, or N, and, optionally, 1-3 addnl. N atoms; or the heteroaryl is a monocyclic ring of 6 atoms, said ring having one heteroatom which is N, and, optionally, 1-4 addnl. N atoms), benzoheteroaryl, NR10R11, SR11, OR11, R11, alkenyl, alkynyl, unsubstituted, mono, di, tri- or tetrasubstituted cycloalkenyl, mono, di, tri- or tetrasubstituted heterocycloalkyl group of 5-7 members, or a benzoheterocycle, wherein said heterocycloalkyl or benzoheterocycle contains 1 or 2 heteroatoms selected from O, S, or N and, optionally, contains a carbonyl group or a sulfonyl group, styryl, mono or disubstituted styryl, phenylacetylene, mono- or disubstituted phenylacetylene, fluoroalkenyl, mono- or disubstituted bicyclic heteroaryl of 8-10 members, containing 2-5 heteroatoms (wherein at least one heteroatom resides on each ring of said bicyclic heteroaryl, said heteroatoms are each independently O, S and N), K, aryl, arylalkyl, cycloalkylalkyl, -C(0)R11, hydrogen, arylalkenyl, arylalkoxy, alkoxy, aryloxy, cycloalkoxy, arylthio, alkylthio, arylalkylthio, or cycloalkylthio. R3 is hydrogen, haloalkyl (preferably CF3), CN, lower alkyl, [C(Re)(Rf)]p-U-V, K, (un) substituted lower alkyl-Q, lower alkyl-O-lower alkyl-Q, etc., Q, alkylcarbonyl, arylcarbonyl, alkylarylcarbonyl, arylalkylcarbonyl, carboxylic ester, carboxamido, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, alkenyl, alkynyl, arylalkyl, lower alkyl-OD1, alkoxyalkyl, aminoalkyl, lower alkyl-CO2R10, lower alkyl-C(O)NR10(R10'), heterocyclic alkyl, or heterocyclic ring-C(O)-; with the proviso that one oxime or hydrazone group must be present; addnl. details are given in the claims.

L4 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:836597 CAPLUS

DOCUMENT NUMBER: 139:317464

TITLE: Amidated derivatives of SR141716A having unique CB1

receptor binding selectivity, and methods for their

production and therapeutic use

INVENTOR(S): Thomas, Brian F.; Seltzman, Herbert H.; Francisco,

Maria Elena Y.

PATENT ASSIGNEE(S): Research Triangle Institute, USA

SOURCE: U.S. Pat. Appl. Publ., 28 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
US 2003199536	A1 20031023	US 2002-121708	20020415
US 6825209	B2 20041130		
WO 2003088968	A1 20031030	WO 2003-US10470	20030414
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ,	CA, CH, CN,
CO, CR, CU,	CZ, DE, DK, DM,	DZ, EC, EE, ES, FI, GB,	GD, GE, GH,
GM, HR, HU,	ID, IL, IN, IS,	·JP, KE, KG, KP, KR, KZ,	LC, LK, LR,
LS, LT, LU,	LV, MA, MD, MG,	MK, MN, MW, MX, MZ, NO,	NZ, OM, PH,
PL, PT, RO,	RU, SC, SD, SE,	SG, SK, SL, TJ, TM, TN,	TR, TT, TZ,
UA, UG, UZ,	VC, VN, YU, ZA,	ZM, ZW	
RW: GH, GM, KE,	LS, MW, MZ, SD,	SL, SZ, TZ, UG, ZM, ZW,	AM, AZ, BY,
KG, KZ, MD,	RU, TJ, TM, AT,	BE, BG, CH, CY, CZ, DE,	DK, EE, ES,

FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1494673 A1 20050112 EP 2003-719602 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.: US 2002-121708 A 20020415

WO 2003-US10470 20030414

OTHER SOURCE(S):

MARPAT 139:317464

443141-84-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(amidated derivs. of SR141716A with unique CB1 receptor binding selectivity, and methods for production and therapeutic use)

RN 443141-84-2 CAPLUS

1H-Pyrazole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-CN hydroxy-4-methyl- (9CI) (CA INDEX NAME)

GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- Compds. are provided that are amide analogs of SR141716A having unique CB1 AB receptor selectivity and providing WIN-sparing binding characteristics. Also provided are pharmaceutical compns. containing the compds. and their use in a method of treatment of CB1 receptor related disorders, e.g. obesity, schizophrenia, memory dysfunction, and marijuana abuse. Compds. of the invention include I [C7-12 (un)branched hydrocarbyl] and II [C7-12 (un) branched hydrocarbyl, N-piperidinyl].

ANSWER 6 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:372410 CAPLUS

DOCUMENT NUMBER: 137:103401

Synthesis and Structure-Activity Relationships of TITLE:

Amide and Hydrazide Analogues of the Cannabinoid CB1

Receptor Antagonist N-(Piperidinyl) -

5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-4-methyl-1H-

pyrazole-3-carboxamide (SR141716)

Francisco, Ma. Elena Y.; Seltzman, Herbert H.; AUTHOR (S):

Gilliam, Anne F.; Mitchell, Rene A.; Rider, Sharyl L.; Pertwee, Roger G.; Stevenson, Lesley A.; Thomas, Brian

CORPORATE SOURCE: Chemistry and Life Sciences Research Triangle

SOURCE:

Institute, Research Triangle Park, NC, 27709, USA

Journal of Medicinal Chemistry (2002), 45(13),

2708-2719

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:103401

443141-84-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and structure-activity relationships of amide and hydrazide analogs of CB1 antagonist SR141716)

443141-84-2 CAPLUS RN

1H-Pyrazole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-CN hydroxy-4-methyl- (9CI) (CA INDEX NAME)

Analogs of the biaryl pyrazole N-(piperidinyl)-5-(4-chlorophenyl)-1-(2,4-AB dichlorophenyl)-4-methyl-1H-pyrazole-3-carboxamide, SR141716 (I) were synthesized to investigate the structure-activity relation (SAR) of the aminopiperidine region. The structural modifications include the substitution of alkyl hydrazines, amines, and hydroxyalkylamines of varying lengths for the aminopiperidinyl moiety. Proximity and steric requirements at the aminopiperidine region were probed by the synthesis of analogs that substitute alkyl hydrazines of increasing chain length and branching. The corresponding amide analogs were compared to the hydrazides to determine the effect of the second nitrogen on receptor binding affinity. The N-cyclohexyl amide (II) represents a direct methine for nitrogen substitution for I, reducing the potential for heteroatom interaction, while the morpholino analog adds the potential for an addnl. heteroatom interaction. The series of hydroxyalkyl amides of increasing chain length was synthesized to investigate the existence of addnl. receptor hydrogen binding sites. In displacement assays using the cannabinoid agonist [3H] (1R, 3R, 4R) - 3 - [2 - hydroxy - 4 - (1, 1 dimethylheptyl)phenyl]-4-(3-hydroxypropyl) cyclohexan-1-ol (CP 55 940) or the antagonist [3H]I,II exhibited the highest CB1 affinity. In general, increasing the length and bulk of the substituent was associated with increased receptor affinity and efficacy (as measured in a GTP-γ-[35S] assay). However, in most instances, receptor affinity and efficacy increases were no longer observed after a certain chain length was reached. A quant. SAR study was carried out to characterize the pharmacophoric requirements of the aminopiperidine region. This model indicates that ligands that exceed 3 Å in length would have reduced potency and affinity with respect to I and that substituents with a pos.

charge d. in the aminopiperidine region would be predicted to possess increased pharmacol. activity.

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 7 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:151538 CAPLUS

DOCUMENT NUMBER: 136:195652

Preparation of pesticidal 1-arylpyrazole oxime TITLE:

derivatives.

Wu, Tai-Teh; Chene, Alain; Manning, David Treadway; INVENTOR(S):

Newsome, Peter Wyatt; Ray, Nicholas Charles; Phillips,

Jennifer Lantz; Lowder, Patrick Doyle

Rhone-Poulenc, Inc., USA PATENT ASSIGNEE(S):

U.S., 31 pp., Cont.-in-part of U.S. Ser. No. 946,375, SOURCE:

abandoned. CODEN: USXXAM

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6350771	<b>B1</b>	20020226	US 1997-989247	19971212
ES 2179386	Т3	20030116	ES 1997-953852	19971218
ZA 9711534	Α	19980624	ZA 1997-11534	19971222
EG 21703	Α	20020227	EG 1997-1391	19971224
TW 476757	В	20020221	TW 1997-86119724	19980302
CN 1316424	Α .	20011010	CN 2001-111650	20010312
US 2002045758	<b>A1</b>	20020418	US 2001-970667	20011005
US 6500850	B2	20021231		
US 2003144251	A1	20030731	US 2002-196959	20020718
US 6638956	B2	20031028		
PRIORITY APPLN. INFO.:			US 1996-33888P P	19961224
			US 1997-946375 B	2 19971007
			US 1997-989247 A	3 19971212
			US 1999-450450 B	1 19991130
			US 2001-970667 A	3 20011005

OTHER SOURCE(S): MARPAT 136:195652 194941-29-2P 194941-31-6P 194941-33-8P 209965-42-4P 209965-45-7P 209965-47-9P 209965-48-0P 209965-49-1P 209965-50-4P 209965-51-5P 209965-52-6P 209965-61-7P 209965-65-1P 209965-68-4P 209965-75-3P 209965-76-4P 209965-80-0P 209965-81-1P 209965-82-2P 209965-83-3P 209965-84-4P 209965-85-5P 209965-86-6P 209965-87-7P 209965-88-8P 209965-89-9P 209965-92-4P 209965-93-5P 209965-96-8P 209965-97-9P 209965-98-0P 209965-99-1P 209966-00-7P 209966-01-8P 209966-02-9P 209966-03-0P 209966-04-1P 209966-05-2P 209966-06-3P 209966-07-4P 209966-08-5P 209966-09-6P

> RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Bio study); PREP (Preparation); USES (Uses)

(preparation as systemic insecticide)

RN 194941-29-2 CAPLUS

401612-77-9P

1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-CN

(trifluoromethyl)phenyl]-N-hydroxy-4-(methylthio)- (9CI) (CA INDEX NAME)

RN 194941-31-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 194941-33-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 209965-42-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-45-7 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-47-9 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(methylamino)-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-48-0 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N N C1 NH2 
$$C1$$

RN 209965-49-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

HO- N=CH 
$$N$$
  $N$   $C1$   $CF_3$   $NH_2$   $N$ 

RN 209965-50-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(trifluoromethyl)thio]-, oxime (9CI) (CA INDEX NAME)

HO-N=CH 
$$N$$
  $CI$   $CF_3$   $NH_2$ 

RN 209965-51-5 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(difluoromethyl)thio]-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N CI 
$$CF_3$$
 $F_2CH-S$   $NH_2$ 

RN 209965-52-6 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylthio)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N CI 
$$CF_3$$
MeS  $NH_2$ 

RN 209965-61-7 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfonyl)-, oxime (9CI) (CA INDEX NAME)

RN · 209965-65-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-68-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(hydroxyimino)methyl]-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

RN 209965-75-3 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-methyl-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-76-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-methyl-4-(methylsulfonyl)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N CF3

Me-
$$s$$
=0 Me

RN 209965-80-0 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2-chloro-4-(trifluoromethyl)phenyl]-5-[[2-(ethylsulfonyl)ethyl]amino]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-81-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-4-(methylthio)-, oxime (9CI) (CA INDEX NAME)

RN 209965-82-2 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-(ethylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-83-3 CAPLUS
CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4(trifluoromethyl)phenyl]-4-(trifluoromethyl)-, oxime (9CI) (CA INDEX

HO-N=CH N C1 
$$CF_3$$

RN 209965-84-4 CAPLUS

NAME)

CN Ethanone, 1-[5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-1H-pyrazol-3-yl]-, oxime (9CI) (CA INDEX NAME)

RN 209965-85-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-86-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylthio)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-87-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-88-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-89-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfonyl)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-92-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(2-fluoroethyl)sulfinyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-93-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(2-fluoroethyl)sulfonyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-96-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-(methylamino)-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-97-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-98-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-[[2-(ethylsulfonyl)ethyl]amino]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-99-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-[(2-cyanoethyl)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH & C1 & CF_3 \\ \parallel & N & \\ Me-s & NH-CH_2-CH_2-CN \\ \downarrow & O \end{array}$$

RN 209966-00-7 CAPLUS

CN Acetamide, 2-[[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3[(hydroxyamino)iminomethyl]-4-(methylsulfinyl)-1H-pyrazol-5-yl]amino](9CI) (CA INDEX NAME)

RN 209966-01-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-[[2-(phenylsulfonyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 209966-02-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dibromo-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209966-03-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2-bromo-6-chloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-(methylsulfinyl)-(9CI) (CA INDEX NAME)

RN 209966-04-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2-bromo-6-chloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209966-05-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-N-hydroxy-5-[[2-(methylsulfinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 209966-06-3 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-[[2-(methylsulfinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 209966-07-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-5-[[2-(ethylsulfinyl)ethyl]amino]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209966-08-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-(2-propynylamino)- (9CI) (CA INDEX NAME)

RN 209966-09-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2-chloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH & CF_3 \\ HO-NH-C & N\\ Me-S & NH_2 \\ \\ O \end{array}$$

RN 401612-77-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-formyl-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

Ι

GI

AB The 1-arylpyrazole oxime derivs. I [X = SOmR6; Z = (un)substituted NH2; R1 = H, alkyl or substituted NH2; R2 = H or halo; R3, R5 = R2 or alkyl; R4 = halo, haloalkyl, haloalkoxy, etc.; R6 = alkyl, haloalkyl, alkenyl, etc.; m = 0, 1 or 2; M = C-halo, C-CH3, C-CH2F, C-CH2Cl or C-NO2] an their geometric isomers and tautomers are prepared as safe systemic insecticides, also useful for control of arthropod, nematode, helminth or protozoan pests.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:423412 CAPLUS

DOCUMENT NUMBER: 135:30294

TITLE: Synergistic insecticidal compositions containing

oxadiazoline derivatives, insect control, and

enhancement of insecticidal action of the derivatives

INVENTOR(S): Akayama, Atsuo

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 67 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

KIND	DATE	APPLICATION NO.	DATE
A2	20010612	JP 1999-340604	19991130
		JP 1999-340604	19991130
			A2 20010612 JP 1999-340604

OTHER SOURCE(S): MARPAT 135:30294

IT 230643-13-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of insecticidal oxadiazoline derivs. and synergistic agrochem. insecticides containing them)

RN 230643-13-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-ethyl-N'-hydroxy-4-[(trifluoromethyl)sulfinyl]-(9CI) (CA INDEX NAME)

GI

Insecticidal compns. contain the derivs. I [R1 = C1-6 alkyl, C1-6 AΒ haloalkyl; n = 0, 1, 2; X = NR2R3 (R2, R3 = H, C1-6 alkyl which may be substituted with pyridyl), N:CHOR4 (R4 = C1-6 alkyl), N:CHNR6R7 (R6, R7 = H, C1-6 alkyl), N:CHAr (Ar = Ph which may be substituted with OH or C1-3 alkoxy), pyrrolyl; R5 = (un)substituted alkyl, (un)substituted acyl; R8 = halo, C1-6 haloalkyl, C1-6 haloalkoxy, Ph which may be substituted with C1-6 haloalkyl; A = N, CR9 (R9 = Cl, cyano); B = N, CH] or their salts and other agrochem. components such as insecticidal clothianidin, nitenpyram, cartap hydrochloride, bensultap, pyraclofos, etc. Insects are controlled by combined use of I or their salts with the other agrochem. components. Insecticidal activity of I or their salts is enhanced by combined use with the other agrochem. components. I (n =1, R1 = R8 = CF3, R5 = CONMe2, A = CCl, B = N, X = N:CHOCHMe2) (preparation given) and clothianidin showed synergistic action against Plutella maculipennis larvae in pot culture of cabbage. Agrochem. formulations containing I were also given.

ANSWER 9 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

2001:421116 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 135:30293

Ι

Ectoparasiticides containing oxadiazoline derivatives TITLE:

and control of ectoparasites in mammals

INVENTOR(S): Akayama, Atsuo

Takeda Chemical Industries, Ltd., Japan PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 63 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
JP 2001158786	A2	20010612	JP 1999-340605	19991130	
PRIORITY APPLN. INFO.:			JP 1999-340605	19991130	

OTHER SOURCE(S): MARPAT 135:30293

230643-13-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxadiazoline derivs. as ectoparasiticides for mammals)

RN 230643-13-7 CAPLUS

1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-CN

(trifluoromethyl)phenyl]-N-ethyl-N'-hydroxy-4-[(trifluoromethyl)sulfinyl]-(9CI) (CA INDEX NAME)

GI

Ectoparasites, e.g. arachnids, flies, lice, fleas, etc., are controlled by AΒ administration of the derivs. I [R1 = C1-6 alkyl, C1-6 haloalkyl; n = 0, 1, 2; X = NR2R3 (R2, R3 = H, C1-6 alkyl which may be substituted with pyridyl), N:CHOR4 (R4 = C1-6 alkyl), N:CHNR6R7 (R6, R7 = H, C1-6 alkyl), N:CHAr (Ar = Ph which may be substituted with OH or C1-3 alkoxy), pyrrolyl; R5 = (un)substituted alkyl, (un)substituted acyl; R8 = halo, C1-6 haloalkyl, C1-6 haloalkoxy, Ph which may be substituted with C1-6 haloalkyl; A = N, CR9 (R9 = Cl, cyano); B = N, CH] or their salts to mammals. I (X = N: CHOEt, N = 1, R1 = R8 = CF3, R5 = CONMe2, A = CC1, B = N) was prepared Emulsions, feed additive granules, oral liqs., injections, aerosols, etc. containing I were also formulated.

ANSWER 10 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

2001:416911 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 135:33474

Control of arthropods in animals using parasiticidal, TITLE:

non-emetic 1-arylpyrazole derivatives

Huber, Scot Kevin; Chou, David Teh-Wei; Schnatterer, Stefan; Bastiaans, Henricus Maria Martinus INVENTOR(S):

PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

INT · 1

PATENT INFORMATION:

PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
WO	WO 2001040195			A2 20010607			WO 2000-EP12100						20001201				
WO	2001	0401	95		A3		2001	1108									
	W:	ΑE,	AG,	AL,	AM,	AU,	AZ,	BA,	BB,	BG	, BR,	BY,	ΒZ,	CA,	CN,	CR,	CU,
		CZ,	DM,	DZ,	EE,	GD,	GE,	HR,	HU,	ID	, IL,	IN,	IS,	JP,	KG,	KP,	KR,
		ΚZ,	LC,	LK,	LR,	LT,	LV,	MA,	MD,	MG	, MK,	MN,	MX,	NO,	NZ,	PL,	RO,
		RU,	SG,	SI,	SK,	ΤJ,	TM,	TT,	UA,	UZ	, VN,	ΥU,	ZA,	AM,	AZ,	BY,	KG,
		KZ,	MD,	RU,	TJ,	TM											
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ,	UG,	ZW,	ΑT,	ΒE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT	, LU,	MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML	, MR,	ΝE,	SN,	TD,	TG		
CA	2393	197			AA		2001	0607		CA	2000-	2393	197		2	0001	201
EP	1237	873			A2		2002	0911	:	EΡ	2000-	9932	56		2	0001	201
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,						, TR						
BR	2000	0159	45		A		2002	1112	:	BR	2000-	1594	5		2	0001	201
	2003						2003	0520		JP	2001-	5418	80		2	0001	201
US	2002						2002	0815	•	US	2000-	7276	84		2	0001	204
	6569				B2		2003										
ZA	2002	0043	36		Α		2003	0320		ZA	2002-	4336			2	0020	530
US	2003	1764	66		A1		2003	0918	•	US	2003-	4064	91		2	0030	404
PRIORIT	Y APP	LN.	INFO	.:					•	US	1999-	1686	58P		P 1	.9991	202
									1	WO	2000-	EP12	100	,	W 2	20001	201
									,	US	2000-	7276	84		A3 2	20001	204

OTHER SOURCE(S): MARPAT 135:33474

IT 343347-31-9P 343347-33-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(parasiticide candidate; preparation of arylpyrazole derivs. as non-emetic parasiticides for arthropod control)

RN 343347-31-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 4-[(chlorodifluoromethyl)thio]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N,5-dihydroxy- (9CI) (CA INDEX NAME)

RN 343347-33-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N,5-dihydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

GI

$$R^{202}$$
  $R^{201}$   $F_{3}C-S$   $CN$ 
 $R^{204}$   $N$ 
 $R^{211}$   $C1$ 
 $R^{213}$   $I$ 
 $R^{214}$   $CF_{3}$   $II$ 

A method of controlling parasites in or on an animal is disclosed, which AB comprises administration of a parasiticidally effective, substantially non-emetic 1-arylpyrazole of formula I [R201 = cyano, alkanoyl, (un) substituted CSNH2 or CONH2, haloalkyl, (un) substituted heterocyclyl, etc.; R202 = S00-2R203, alkenyl, alkynyl, cycloalkyl, NO2, (un)substituted imidazolyl, etc.; R203 = alkyl, haloalkyl; R204 = OH or numerous derivs.; X1 = N, CR212; R211, R212 = H, halo, cyano, C1-3 alkyl, NO2; R213 = halo, haloalkyl, haloalkoxy, SO0-2CF3, SF5; R214 = H; or R213R214 = OCF20, CF2OCF2, CF2OCF2O, CF2CF2O], or a veterinarily acceptable salt. The compds. are particularly useful in domestic animals, most preferably dogs and cats, and preferably by oral administration.. The parasites which are controlled are particularly ectoparasites, and preferably fleas and ticks. I are advantageous by virtue of reduced emesis. Several large tables of compds. I are listed, with phys. data for approx. 50 compds. instance, oxidation of the known compound 1-(2,6-dichloro-4trifluoromethylphenyl)-3-cyano-4-trifluoromethylsulfenyl-5-hydroxypyrazole [II; n = 0] with m-chloroperbenzoic acid gave 37% II [n = 1]. Alternatively, oxidation of II [n = 0] using peracetic acid gave 50.2% II [n = 2]. When fed to cats at 20 mg/kg, and dogs at 10 mg/kg, and formulated at 30 mg/mL in 1:1 (volume/volume) DMSO and corn oil, II [n = 1, 2] and other selected I gave satisfactory control of the flea Ctenocephalides felis and the tick Rhipicephalus sanguineus, without any significant side effects. Potential application to control of arthropod and nematode pests of plants is also mentioned.

L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:784098 CAPLUS

DOCUMENT NUMBER: 132:12312

TITLE: Preparation of (phenylpyrazolyl)oxadiazolines and

analogs as insecticides

INVENTOR(S): Kando, Yasuyuki; Noguchi, Makoto; Akayama, Atsuo;

Masada, Shinichi; Kiji, Toshiyuki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

						KIND DATE													
								1999									9990!	531	
								BA,											
			•		•			IN,	•			•							
		-	MD,	MG,	MK,	MN,	MX,	NO,	ΝZ,	PL,	RO,	RU,	SG,	SI,	SK,	SL,	ТJ,	TM,	
			TR,	TT,	UA,	US,	UΖ,	VN,	YU,	ZA,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM
		RW:	GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ,	ŬĠ,	ZW,	ΑT,	BE,	CH,	CY,	DE,	DK,	
			ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	
			CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG						
C	CA 2	23337	759			AA		1999	1209		CA 1	999-	2333	759		1	9990	531	
F	UA	99395	573			A1		1999	1220		AU 1	999-	3957	3		1	9990	531	
								2000											
E	3R 9	99109	912			Α		2001	0306		BR 1	999-	1091	2		1	9990	531	
								2001											
						В1		2002											
_								ES,	FR.	GB.	GR.	IT.	LI.	LU.	NL.	SE.	MC.	PT.	
				FI		,		,	•	,	,		•		•	•	•	•	
7	νт :	22152	29			E		2002	0815		AT 1	999-	9225	86		1	9990	531	
		21772				T3		2002											
		11318				В		2003											
-						В		2004			-								
						B1		2001											
PRIORI						בט		2001	0711				1531						
FKIOKI	LII	APPI	T17.4	TMLO	• •								2347						
													9555						
													JP28						
											MO I	フフファ	0220	70		AA T	<b>フ</b> フフロ	33 I	

OTHER SOURCE(S): MARPAT 132:12312

IT 230643-13-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oxadiazoline derivs. and their use as insecticides)

RN 230643-13-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-

(trifluoromethyl)phenyl]-N-ethyl-N'-hydroxy-4-[(trifluoromethyl)sulfinyl](9CI) (CA INDEX NAME)

GI

AB Title compds. [I; R = NR2R3, N:CHOR4, N:CHPh, etc.; R1 = (halo)alkyl; R2,R3 = H, (pyridyl)alkyl; R4 = alkyl; R5 = (un)substituted alkyl, -acyl; Z = N or CH; Z1 = SOO-2; Z2 = N or CR9; R9 = Cl or cyano] were prepared Thus, I (R = NH2, Z1R1 = SO2CF3, R8 = CF3, Z = N, Z2 = CCl)(II; R5 = H) was condensed with HC(OCHMe2)3 to give II [R5 = (Me2CHO)2CH]. Data for biol. activity of I were given.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:409212 CAPLUS

DOCUMENT NUMBER: 131:98844

TITLE: Control of pests in containerized seedlings with

nitrogen-containing insecticides

INVENTOR(S): Akayama, Atsuo

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 117 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATĖ	APPLICATION NO.	DATE
JP 11171702 PRIORITY APPLA	A2		JP 1998-264372 JP 1997-258947	
OTHER SOURCE(S): IT 185615-32-1 185617				
194941-31-6 194941 194941-37-2 194941				
194941-53-2 194941 194941-58-7 194941				
194941-61-2 194941 194941-64-5 194941				
194941-82-7 194941	-83-8		logical study); USES	(Hees)
(insecticide fo	r contai			(USES)
RN 185615-32-1 CAPLU CN 1H-Pyrazole-3-carb	<del>-</del>	nide, 5-amino	o-1-[2,6-dichloro-4-	

(trifluoromethyl)phenyl]-N-hydroxy-4-(2,2,2-trifluoro-1-hydroxyethyl)(9CI) (CA INDEX NAME)

RN 185617-32-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(2,2,2-trifluoro-1-hydroxy-1-methylethyl)- (9CI) (CA INDEX NAME)

HO-NH-C-Me NH<sub>2</sub>

$$F_3C-C-Me$$
NH
C1
$$CF_3$$

$$CT_3$$

$$CT_3$$

RN 194941-29-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylthio)- (9CI) (CA INDEX NAME)

RN 194941-31-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 194941-33-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-36-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO- NH- C NH2 CF3

$$r_3$$
 C- S O NH2

RN 194941-37-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO-NH-C NH<sub>2</sub> C1 CF<sub>3</sub> 
$$R_{3}$$
 C1  $R_{1}$  C1  $R_{2}$  CF<sub>3</sub>

RN 194941-49-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO-NH-C NMe<sub>2</sub> 
$$CF_3$$

RN 194941-51-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

RN 194941-53-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

RN 194941-55-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

HO-NH-C NMe<sub>2</sub> 
$$CF_3$$
  $CF_3$ 

RN 194941-57-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-58-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-59-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(1-methylethyl)amino]-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-60-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(phenylmethyl)amino]-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

HO-NH-C NH-CH<sub>2</sub>-Ph

$$F_3C-S$$
 $NH-CH_2-Ph$ 

RN 194941-61-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-[bis(phenylmethyl)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

HO-NH-C N CF3

$$F_3C-S$$
 N-CH2-Ph

 $CF_3$ 
 $CF_3$ 

RN 194941-62-3 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-(methylamino)-4-[(trifluoromethyl)sulfonyl]-(9CI) (CA INDEX NAME)

HO-NH-C NHMe

$$F_3C-S=0$$
 NHMe

 $C1$ 
 $CF_3$ 

RN 194941-63-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO-NH-C NMe<sub>2</sub> 
$$CF_3$$
  $CF_3$ 

RN 194941-64-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO-NH-C NHET

$$F_3C-S=0$$

NHET

 $CF_3$ 
 $CF_3$ 

RN 194941-65-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO-NH-C N N C1 CF3
$$F_3C-S=0 NEt_2$$

RN 194941-81-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-[[(ethylamino)carbonyl]amino]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]-(9CI) (CA INDEX NAME)

RN 194941-82-7 CAPLUS

CN Benzamide, N-[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3[(hydroxyamino)iminomethyl]-4-[(trifluoromethyl)sulfonyl]-1H-pyrazol-5-yl](9CI) (CA INDEX NAME)

HO- NH- C NH C1 CF3

$$F_3C-S=0$$
 NH C1 C- Ph

RN 194941-83-8 CAPLUS

CN Benzamide, N-[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3[(hydroxyamino)iminomethyl]-4-[(trifluoromethyl)sulfinyl]-1H-pyrazol-5-yl](9CI) (CA INDEX NAME)

IT 230643-13-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of)

RN 230643-13-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-ethyl-N'-hydroxy-4-[(trifluoromethyl)sulfinyl]-(9CI) (CA INDEX NAME)

$$Et-N = C$$

$$F_3C-S$$

$$NH_2$$

$$NH_2$$

AB A labor-saving method for controlling pests in angiosperms, except Gramineae, involves raising seedlings in a container filled with medium that, before seeding or temporary planting, is mixed with an insecticide of the formula R1R2NCR3:Y, where R1 = H, hydrocarbon, acyl, or substituted alkyl, the substituent possibly being heterocyclic; R2 = H, hydrocarbon, or a bivalent group bound to R3; R3 = hydrocarbon, SR4 (where R4 has the same meanings as R1), or YR5R6 (where R5 and R6 are the same or different and have the same meanings as R1), etc.; Y = :N or :CZ, where Z = H or hydrocarbon, optionally substituted; and X = electron-withdrawing substituent. Thus, in a pot experiment with cucumber, mixing granules containing

1-N-[(6-chloro-3-pyridylmethyl)-N-ethylamino]-1-methylamino-2-nitroethylene at 0.286 g/L with medium completely controlled Aphis gossypii.

L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:279733 CAPLUS

DOCUMENT NUMBER: 130:311789

TITLE: Preparation of pesticidal 3-substituted arylpyrazoles

INVENTOR(S): Wu, Tai-Teh

PATENT ASSIGNEE(S): Rhone-Poulenc Agro, Fr. SOURCE: Eur. Pat. Appl., 40 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT 1	10.		KINI	)	DATE		APPLICATION NO.						DATE				
	 29		7.7	•	1000	0420		1000	1104				10000	020			
							EP										
R:	AT, BE,	CH,	DE,	DK	, ES,	FR,	GB, GI	R, IT,	LI,	LU,	ΝL,	SE	E, MC,	PT,			
	IE, SI,	LT,	LV,	FI	, RO												
US 5981	565		Α		1999	1109	US	1997-	9461	32			19971	007			
US 6008	353		Α		1999	1228	US	1997-	9460	54			19971	007			
US 6107	314		Α		2000	0822	US	1997-	9466	48			19971	007			
JP 1126	3777		<b>A2</b>		1999	0928	JP	1998-	2830	56			19981	005			
US 6432	997		B1		2002	0813	US	1999-	4048	09			19990	924			
US 6277	348		<b>B</b> 1		2001	0821	US	1999-	4408	50			19991	116			
US 6346	522		B1		2002	0212	US	1999-	4408	49			19991	116			
US 6376	520		B1		2002	0423	US	2001-	9309	46			20010	817			
US 2002	173492		A1		2002	1121	US	2002-	6022	9			20020	201			
US 6500	848		B2		2002	1231											
US 2003	092680		A1		2003	0515	US	2002-	2389	02			20020	911			
US 6593	328		B2		2003	0715											
PRIORITY APP	LN. INFO	. :					US	1997-	9460	54		Α	19971	007			
							US	1997-	9461	32		Α	19971	007			
							US	1997-	9466	48		Α	19971	007			
							US	1999-	4408	50		А3	19991	116			
							US	2001-	9309	46		<b>A</b> 3	20010	817			
						•							20020				

OTHER SOURCE(S):

MARPAT 130:311789

IT 209965-87-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pesticidal 3-substituted arylpyrazoles)

RN 209965-87-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

GΙ

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I; R1 = II-IV (R1a = H, alkyl, a lone pair of electrons; R1b = alkyl, aryl; X = O, NH, N(alkyl); Q = CR8R9, C(:Y), etc.; R8, R9 = H, alkyl, aryl, etc.; Y = O, S; Z = alkyl, aryl; W = H, alkyl, alkenyl, etc.; V = H, alkyl, CN, etc.); R2 = alkyl, haloalkyl, SOnR2a (R2a = alkyl, alkenyl, alkynyl, etc.); R3 = H, halo, alkyl, etc.; R4, R5, R7 = H, halo, alkyl; R6 = halo, haloalkyl, haloalkoxy, etc.; M = C(halo), C(Me), N, etc.], having pesticidal activity, were prepared Thus, reaction

of 5-amino-1-(2,6-dichloro-4-trifluoromethylphenyl)-4-methylsulfinyl-3-[3-(1-amidoxime)]pyrazole (preparation given) with trifluoroacetic anhydride in dioxane afforded the title compound V which showed insecticidal activity in one or more of the evaluation methods (described in patent), with

particularly good activity in the systemic tests.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:244518 CAPLUS

DOCUMENT NUMBER: 130:248363

TITLE: Insecticidal 3-cyanopyrazole derivatives.

INVENTOR(S): Wu, Tai-Teh

PATENT ASSIGNEE(S): Rhone-Poulenc Agro, Fr. SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.						KIND DATE				APPL	ICAT:		DATE				
							-									-		
	WO	9917	613			<b>A1</b>		1999	0415	1	WO 1:	998-1	EP66	58		1	9981	005
		W:	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
			DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IS,	JP,	KΕ,	KG,
•			ΚP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,
	NO, NZ, PL,			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	
			UA,	UG,	US,	UΖ,	VN,	YU,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	DK,	ES,
			FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,
			CM,	GΑ,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG						
	ΑU	9910	311			<b>A1</b>		1999	0427		AU 1	999-:	1031	1		1	9981	005
PRIOR	RIORITY APPLN. INFO.:			. :					•	US 1	997-	6124	4 P	:	P 1	9971	007	
									•	US 1	997-	6226	9P	:	P 1	9971	017	
										1	WO 1	998-1	EP66	58	1	W 1	9981	005

OTHER SOURCE(S): MARPAT 130:248363

IT 194941-33-8 209965-87-7

RL: AGR (Agricultural use); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(insecticide)

RN 194941-33-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 209965-87-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-

(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI)

GI

AB Known 3-cyanopyrazole insecticides are delivered to a locus by application of their derivs. I [X = group bonded through N, O or S; Y = H or a group bonded through C, N, O, S or P; XY = YN:CX; W = halo or a group bonded through C, N, O, S or P; R = H or W; Ar = (un) substituted aryl or heteroaryl]. I are converted spontaneously on the locus into the corresponding active 3-cyanopyrazole derivs.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS. RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 15 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1999:9820 CAPLUS

DOCUMENT NUMBER:

130:81510

TITLE:

Preparation of phenylpyrazolecarboxamides as

coagulation factor Xa inhibitors

INVENTOR (S):

Galemmo, Robert Anthony, Jr.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Lam, Patrick Yuk-sun; Pinto, Donald Joseph Philip; Pruitt, James Russell; Quan,

Mimi Lifen

PATENT ASSIGNEE(S):

The Du Pont Merck Pharmaceutical Company, USA

SOURCE:

PCT Int. Appl., 259 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIN	D	DATE			APPL	ICAT:	ION I	NO.		DATE			
						-									-			
WO	9857	937			A2		1998	1223	1	WO 1	998-1	US12	681		1	9980	618	
WO	9857	937			A3		1999	0318										
	W:	AU,	BR.	CA.	CN.	CZ.	EE.	HU.	IL.	JP.	KR.	LT,	LV.	MX.	NO.	NZ.	PL.	

		RO,	SG,	SI,	SK,	UA,	VN,	AM,	AZ,	BY	, KG,	KZ,	MD,	RU,	ТJ,	TM	
	RW:	ΑT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR	, GB,	GR,	ΙE,	IT,	LU,	MC,	NL,
		PT,	SE														
ZA	9805	251			Α		1999	1217	2	ZA	1998-	5251			1	9980	617
CA	2290	982			AA		1998	1223	(	CA	1998-	2290	982		1	9980	618
AU	9881	503			<b>A1</b>		1999	0104	1	UA	1998-	8150	3		1	9980	618
US	5998	424			Α		1999	1207	τ	US	1998-	9975	2		1	9980	618
EP	9916	25			A2		2000	0412	I	EΡ	1998-	9313	55		1	9980	618
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	PT,	ΙE,
		SI,	LT,	LV,	FI,	RO											
BR	9810	151			Α		2000	8080	1	BR	1998-	1015	1		1	9980	618
EE	9900	584			Α		2000	0815	1	EE	1999-	584			1	9980	618
SI	2020	8			С		2000	1031	5	SI	1998-	2004	3		1	9980	618
JP	2002	5079	68		T2		2002	0312	Ċ	JP	1999-	5047	86		1	9980	618
US	6403	620			В1		2002	0611	τ	US	1999-	3937	82		1	9990	910
LV	1251	6			В		2001	0320	]	LV	1999-	177			1	9991	216
NO	9906	316			Α		1999	1217	1	NO	1999-	6316			1	9991	217
LT	4702				В		2000	0925	]	LT	1999-	146			1	9991	217
US	2003	0927	40		A1		2003	0515	Ţ	US	2002-	1506	98		2	0020	516
US	6602	895			B2		2003	0805									
PRIORITY	Y APP	LN.	INFO	. :					τ	US	1997-	5021	9P		P 1	9970	619
									Ţ	US	1997-	8788	85		A 1	9970	619
									τ	US	1998-	7669	1P		P 1	.9980	227
									τ	US	1998-	9975	2		A3 1	.9980	618
									1	WO	1998-	US12	681		W 1	9980	618
									1	US	1999-	3937	82		A3 1	9990	910

OTHER SOURCE(S):

MARPAT 130:81510

IT 218631-16-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylpyrazolecarboxamides as coagulation factor Xa inhibitors)

RN 218631-16-4 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxamide, N3-hydroxy-1-(4-methoxyphenyl)-N5-[4-(1-pyrrolidinylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)

GI ·

AB EZ1M [I; E = halo, OH, alkyl, alkoxy, etc.; M = Z2ZAB; A = (un)substituted carbocyclylene, -heterocyclylene; B = H, Y, XY; X = alkylene, CO, O, (un)substituted NH, etc.; Y = amino(alkyl), substituted carbocyclyl, -heterocyclyl, etc.; Z = bond, (heteroatom- or functional group-interrupted) alkylene, etc.; Z1 = (un)substituted Ph, Z2 = N-containing heteroarylene, etc.] were prepared Thus, MeCOCH2C(:NOMe)CO2Et was cyclocondensed with PhNHNH2 and the product amidated by 4-(H2N)C6H4C6H4(SO2NHCMe3)-2 to give, after deprotection, title compound II. Data for biol. activity of I were given.

L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1998:479511 CAPLUS

DOCUMENT NUMBER:

129:109088

TITLE:

Pesticidal 1-arylpyrazoles

INVENTOR(S):

Chene, Alain; Lowder, Patrick Doyle; Manning, David Treadway; Newsome, Peter Wyatt; Phillips, Jenniver

Lantz; Ray, Nicholas Charles; Wu, Tai-teh

PATENT ASSIGNEE(S):

Rhone-Poulenc Agrochimie, Fr.

SOURCE:

PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PAT	ENT I					KIND DATE			DATE APPLICATION NO.									
WO	9828	278			A1		1998	0702	1	WO 1:	997-1	EP71	17		19	9712	218	
	W:	AL,	AU,	BA,	BB,	BG,	BR,	CA,	CN,	CU,	CZ,	EE,	GE,	GW,	ΗU,	ID,	IL,	
		ıs.	JP,	KP,	KR,	LK,	LR,	LT,	LV,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,	
							TT,											
			TJ,		•	•	•	·	•	•								
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	
		FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	
							SN,											
CA	2275	920			AA		1998	0702		CA 1	997-		19971218					
	9857																	
	7457																	
EΡ	9484	85			A1		1999	1013		EP 1	997-	9538	52		1:	9971	218	
	9484						2002											
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	PT,	ΙE,	
		SI,	LT,	LV,	FI,	RO												
CN	1245	492			Α		2000	0223		CN 1	997-	1816	01		1:	9971	218	
CN	1094	928			В		2002	1127										
BR	9714	187			Α		2002	0229		BR 1	997-	1418	7		1:	9971	218	
EE	9900322						2000	0615	5 EE 1999-322									
EE	E 4306				В1		2004	0615										
JP					Т2				JP 1998-528352						19971218			

```
19971218
     AP 1039
                                 20020123
                                             AP 1999-1589
            KE, MW, SD,
                             ZW
         W :
                         UG,
                                             AT 1997-953852
     AT 224877
                          Ε
                                 20021015
                                                                     19971218
     ES 2179386
                          T3
                                 20030116
                                             ES 1997-953852
                                                                     19971218
                                 20040203
                                             SK 1999-859
                                                                     19971218
     SK 283823
                          B6
                                             ZA 1997-11534
                                                                     19971222
     ZA 9711534
                          Α
                                 19980624
     EG 21703
                          Α
                                 20020227
                                             EG 1997-1391
                                                                     19971224
                          В
                                             TW 1997-86119724
                                                                     19980302
     TW 476757
                                 20020221
                                             BG 1999-103591
                                                                     19990719
     BG 103591
                          Α
                                 20001130
                                 20011010
                                                                     20010312
     CN 1316424
                          Α
                                             CN 2001-111650
                                             US 1996-33888P
                                                                     19961224
PRIORITY APPLN. INFO.:
                                             US 1997-946375
                                                                 A 19971007
                                                                     19971218
                                             WO 1997-EP7117
OTHER SOURCE(S):
                         MARPAT 129:109088
     194941-29-2P 194941-31-6P 194941-33-8P
     194941-36-1P 194941-37-2P 209965-42-4P
     209965-45-7P 209965-47-9P 209965-48-0P
     209965-49-1P 209965-50-4P 209965-51-5P
     209965-52-6P 209965-61-7P 209965-65-1P
     209965-67-3P 209965-68-4P 209965-74-2P
     209965-75-3P 209965-76-4P 209965-78-6P
     209965-79-7P 209965-80-0P 209965-81-1P
     209965-82-2P 209965-83-3P 209965-84-4P
     209965-85-5P 209965-86-6P 209965-87-7P
     209965-88-8P 209965-89-9P 209965-92-4P
     209965-93-5P 209965-96-8P 209965-97-9P
     209965-98-0P 209965-99-1P 209966-00-7P
     209966-01-8P 209966-02-9P 209966-03-0P
     209966-04-1P 209966-05-2P 209966-06-3P
     209966-07-4P 209966-08-5P 209966-09-6P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pesticidal arylpyrazoles)
     194941-29-2 CAPLUS
RN
     1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-
CN
     (trifluoromethyl)phenyl]-N-hydroxy-4-(methylthio)- (9CI) (CA INDEX NAME)
```

RN 194941-31-6 CAPLUS
CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 194941-33-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-36-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO-NH-C NH<sub>2</sub> CF<sub>3</sub>

$$F_3C-S=O NH2$$

$$N$$

$$N$$

$$CT$$

$$CF_3$$

$$N$$

$$C1$$

$$C1$$

RN 194941-37-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO-NH-C NH2 C1 
$$CF_3$$

RN 209965-42-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH 
$$N$$
  $N$   $C1$   $CF_3$   $NH_2$   $NH_2$ 

RN 209965-45-7 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-47-9 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(methylamino)-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-48-0 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N O-CF<sub>3</sub>

$$Me-s NH2$$
NH<sub>2</sub>

RN 209965-49-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-50-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(trifluoromethyl)thio]-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N N C1 
$$F_3C-S$$
  $NH_2$ 

RN 209965-51-5 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(difluoromethyl)thio]-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N N CI 
$$_{\rm F_2CH-S}$$
 NH<sub>2</sub>

RN 209965-52-6 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-

(trifluoromethyl)phenyl]-4-(methylthio)-, oxime (9CI) (CA INDEX NAME)

RN 209965-61-7 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfonyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-65-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-67-3 CAPLUS

CN 1H-Pyrazole-3,5-dicarboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(trifluoromethyl)thio]-, 3-oxime (9CI) (CA INDEX NAME)

HO-N=CH 
$$\sim$$
 Cl  $\sim$  CF3

RN 209965-68-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(hydroxyimino)methyl]-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO- NH- C N CF3

$$F_3C-S$$
 CH N- OH

RN 209965-74-2 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-methyl-4-(methylthio)-, oxime (9CI) (CA INDEX NAME)

RN 209965-75-3 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-methyl-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-76-4 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-methyl-4-(methylsulfonyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-78-6 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylthio)-5-methyl-, oxime (9CI) (CA INDEX NAME)

RN 209965-79-7 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-5-methyl-, oxime (9CI) (CA INDEX NAME)

HO-N=CH
N
N
C1
CF3
$$CF3$$
 $CF3$ 

RN 209965-80-0 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2-chloro-4-(trifluoromethyl)phenyl]-5-[[2-(ethylsulfonyl)ethyl]amino]-4-(methylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-81-1 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-4-(methylthio)-, oxime (9CI) (CA INDEX NAME)

RN 209965-82-2 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-(ethylsulfinyl)-, oxime (9CI) (CA INDEX NAME)

RN 209965-83-3 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(trifluoromethyl)-, oxime (9CI) (CA INDEX NAME)

HO-N=CH N 
$$CF_3$$
  $CF_3$   $CF_3$ 

RN 209965-84-4 CAPLUS

CN Ethanone, 1-[5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-1H-pyrazol-3-yl]-, oxime (9CI) (CA INDEX NAME)

RN 209965-85-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-86-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylthio)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-87-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-88-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-89-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfonyl)-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-92-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(2-fluoroethyl)sulfinyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 209965-93-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(2-fluoroethyl)sulfonyl]-N-hydroxy-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
NH & C1 & CF_3 \\
HO-NH-C & N & C1
\end{array}$$

$$FCH_2-CH_2-S=0 \quad NH_2$$

RN 209965-96-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-(methylamino)-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-97-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-98-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-[[2-(ethylsulfonyl)ethyl]amino]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209965-99-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-[(2-cyanoethyl)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH & C1 & CF_3 \\ \parallel & N & \\ Me^{-S} & NH^{-}CH_2^{-}CH_2^{-}CN \\ \downarrow & O \end{array}$$

RN 209966-00-7 CAPLUS

CN Acetamide, 2-[[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-[(hydroxyamino)iminomethyl]-4-(methylsulfinyl)-1H-pyrazol-5-yl]amino]-(9CI) (CA INDEX NAME)

RN 209966-01-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-[[2-(phenylsulfonyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 209966-02-9 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dibromo-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

. 10/608,333

RN 209966-03-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2-bromo-6-chloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-(methylsulfinyl)-(9CI) (CA INDEX NAME)

RN 209966-04-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2-bromo-6-chloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 209966-05-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-N-hydroxy-5-[[2-(methylsulfinyl)ethyl]amino]-(9CI) (CA INDEX NAME)

RN 209966-06-3 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-[[2-(methylsulfinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 209966-07-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(ethylsulfinyl)-5-[[2-(ethylsulfinyl)ethyl]amino]-N-hydroxy-(9CI) (CA INDEX NAME)

RN 209966-08-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)-5-(2-propynylamino)- (9CI) (CA INDEX NAME)

RN 209966-09-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2-chloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfinyl)- (9CI) (CA INDEX NAME)

GI

The invention relates to novel 1-arylpyrazole oxime derivs. I [X = S(0) mR6 or R7; Y = H, alkenyl, alkynyl, CHO, aroyl, arylsulfonyl, (un)substituted alkyl or haloalkyl; Z = H, halo, COR7, alkyl, S(0) nR8, CHO, CH:NOH, amino, etc.; R1 = H, alkyl, (di) (alkyl) amino; R2 = H, halo; R3, R5 = H, halo, alkyl; R4 = halo, haloalkyl, haloalkoxy, haloalkylthio, -sulfinyl, -sulfonyl, SF5; R6 = (halo)alk(en/yn)yl, cycloalkyl; R7 = alkyl, haloalkyl; R8 = R7, Ph; m, n = 0, 1, 2; N = C-halo, CMe, C(CH2F), C(CH2Cl), C(NO2), or N] and addnl. analogs. The compds. are generally safe systemic insecticides (no data) for control of arthropod, nematode, helminth, or protozoan pests. Also disclosed are compns. and derivs. For

instance, the nitrile 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-1H-pyrazole-3-carbonitrile was reduced to the aldehyde using (iso-Bu)2AlH, and the aldehyde was converted to the oxime with NH2OH.HCl and pyridine, to give title compound II.

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 17 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN L4

ACCESSION NUMBER:

1997:533617 CAPLUS

DOCUMENT NUMBER:

127:220657

TITLE:

Preparation of arylpyrazole insecticides

INVENTOR (S):

Kando, Yasuyuki; Kiji, Toshiyuki; Akayama, Atsuo;

Noguchi, Makoto

PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan; Kando,

Yasuyuki; Kiji, Toshiyuki; Akayama, Atsuo; Noguchi,

Makoto

SOURCE:

PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PAT	CENT 1	10.			KIND DATE								ION 1		DATE				
	WO	9728:	126			A1	-	1997	0807								]	9970	 129	
																		GE,		
			IL,	IS,	KG,	KR,	KZ,	LC,	LK,	LR,	LT	۲,	LV,	MD,	MG,	MK,	MN,	MX,	NO,	
		·																VN,		
								RU,				•		•	•	•	•	•	•	
		RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH	ł,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	
					-		-	•	-	-		-	•					GN,		
			•	•		TD,	•	•	•	•		•		•	•	•	•	•	•	
	ΑU	9715	557 <sup>°</sup>	•	•	A1		1997	0822		ΑU	19	97-	1555	7		1	9970	129	
		10152																		
	ΕP	87922	29			<b>A1</b>		1998	1125		EΡ	19	997-	52	19970129					
		87922																		
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	₹,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,																	
	CN	1210	518			Α												9970		
	BR	97074	473			Α		1999	0727		BR	19	997-	7473			1	9970	129	
		22726				E												9970		
	ES	2187	751			Т3		2003	0616		ES	19	97-	9017	52		1	9970	129	
	US	63164	477			В1		2001	1113		US	19	998-	1172	31		1	9980	724	
PRIOF																		9960	130	
											JP	19	996-2	2562	51	1	A. 1	9960	927	
											WO	19	97-	JP19	0	1	W 1	9970	129	
OTHER	S	URCE	(S):			MAR	PAT	127:	2206	57										
IT	194	941-2	29-21	P 19	4941	-31-	6P 1	9494	1-33	-8P										
	194	941-	36-1	P 19	4941	-37-	2P 1	9494	1-49	-6P										
	194	1941-	51-0	P 19	4941	-53-	2P 1	9494	1-55	-4P										

194941-57-6P 194941-58-7P 194941-59-8P

194941-60-1P 194941-61-2P 194941-62-3P

194941-63-4P 194941-64-5P 194941-65-6P

194941-81-6P 194941-82-7P 194941-83-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylpyrazole insecticides)

194941-29-2 CAPLUS RN

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylthio)- (9CI) (CA INDEX NAME)

RN 194941-31-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 194941-33-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-36-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 194941-37-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO-NH-C NH<sub>2</sub> Cl CF<sub>3</sub> 
$$R_{3}$$
 Cl NH<sub>2</sub>  $R_{3}$ 

RN 194941-49-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

HO-NH-C NMe<sub>2</sub> 
$$CF_3$$

RN 194941-51-0 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

RN 194941-53-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)

RN 194941-55-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-57-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-58-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-59-8 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(1-methylethyl)amino]-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-60-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-[(phenylmethyl)amino]-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

RN 194941-61-2 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-[bis(phenylmethyl)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]- (9CI) (CA INDEX NAME)

HO-NH-C NH-CF3

$$F_3C$$
-S N-CH2-Ph

 $CF_3$ 
 $CF_3$ 

RN 194941-62-3 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-(methylamino)-4-[(trifluoromethyl)sulfonyl]-(9CI) (CA INDEX NAME)

HO-NH-C NHMe

$$C1$$
 $CF_3$ 
 $C_1$ 
 $C_1$ 

RN 194941-63-4 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(dimethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 194941-64-5 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(ethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 194941-65-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-(diethylamino)-N-hydroxy-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 194941-81-6 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-5-[[(ethylamino)carbonyl]amino]-N-hydroxy-4-[(trifluoromethyl)sulfinyl]-(9CI) (CA INDEX NAME)

RN 194941-82-7 CAPLUS

CN Benzamide, N-[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3[(hydroxyamino)iminomethyl]-4-[(trifluoromethyl)sulfonyl]-1H-pyrazol-5-yl](9CI) (CA INDEX NAME)

RN 194941-83-8 CAPLUS

CN Benzamide, N-[1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3[(hydroxyamino)iminomethyl]-4-[(trifluoromethyl)sulfinyl]-1H-pyrazol-5-yl](9CI) (CA INDEX NAME)

IT 194942-39-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of arylpyrazole insecticides)

RN 194942-39-7 CAPLUS

CN 1H-Pyrazole-3-carboxamide, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-5-(methylamino)-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

HO-NH-C NHMe

$$F_3C-S=0$$
 NHMe

IT 194942-34-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of arylpyrazole insecticides)

RN 194942-34-2 CAPLUS

CN 1H-Pyrazole-3-carboxamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy- (9CI) (CA INDEX NAME)

GI

The title compds. [I; Ar = aromatic hydrocarbon group, aromatic heterocyclic AB group; R = H, halo, group bonded through C, N, O, S or P; W = halo, group bonded through C, N, O, S or P; X = H, group bonded through C, N, O or S; Y = H, group bonded through C, N, O, S or P; XY = together with the adjacent nitrogen atom to Y may form an optionally substituted nitrogen-containing heterocyclic group which may further have N, O, S and/or P] which are effective in preventing sanitary or horticultural insect pests and animal and plant parasites and can exert potent insecticidal activities when they are applied to harmed living animals or plants, were prepared Moreover, the compds. I possess safe and advantageous properties as agents for preventing sanitary, horticultural or agricultural injurious insects, such as no substantial damage on plants and less toxicity against Thus, reaction of 5-amino-3-cyano-1-(2,6-dichloro-4trifluoromethylphenyl)-4-methylsulfonylpyrazole with H2NOH.HCl in the presence of Et3N in dioxane afforded 87% I [Ar = 2,6-dichloro-4trifluoromethylphenyl; R = NH2; W = SO2Me; X = NH2; Y = OH] which showed 100% mortality against Chilo suppressalis with no damage to young rice seedlings.

ANSWER 18 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:324628 CAPLUS

DOCUMENT NUMBER: 127:65719

TITLE: Reaction of 4-hydroxy-5-oximino-3-

thiophenecarboxylates with hydrazines. Formation of

pyrazolylthiohydroxamic acids

Robey, R. L.; Alt, C. A.; Van Meter, E. E. AUTHOR (S):

Lilly Research Laboratories, Lilly Corporate Center, CORPORATE SOURCE:

Eli Lilly and Company, Indianapolis, IN, 46285, USA

Journal of Heterocyclic Chemistry (1997), 34(2), SOURCE: 413-428

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal English LANGUAGE:

ΙT 191418-77-6P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazolylthiohydroxamic acids by reaction of hydroxyoximinothiophenecarboxylates with hydrazines)

RN 191418-77-6 CAPLUS

1H-Pyrazole-4-carboxylic acid, 3-[(hydroxyamino)thioxomethyl]-1-phenyl-, CN ethyl ester (9CI) (CA INDEX NAME)

The reactions of 4-hydroxy-5-oximino-3-thiophenecarboxylates with AB hydrazine and substituted hydrazines have been investigated. The product of the reactions have been shown to be pyrazole-3- or 5-thiohydroxamic acids rather than the hydrazones previously described by Benary and Silberstrom (1919). Two alternate mechanisms are proposed which account for the regiochem. outcome. The structures of the pyrazole-3- and 5-thiohydroxamic acids and corresponding nitriles have been proven by independent synthesis, comparison to known compds., and by proton and carbon magnetic resonance and long range HETCOR expts.

REFERENCE COUNT:

THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 19 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

51

1997:72214 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 126:89367

TITLE: Preparation of pyrazole derivatives as insecticides

Kando, Yasuyuki; Kiji, Toshuki; Noguchi, Makoto; INVENTOR(S):

Manabe, Yukiaki

Takeda Chemical Industries Ltd, Japan PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 61 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 08311036	A2	19961126	JP 1996-4929		19960116
PRIORITY APPLN. INFO.:			JP 1995-54820	Α	19950314

MARPAT 126:89367 OTHER SOURCE(S):

185615-33-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrazole derivs. as insecticides)

RN185615-33-2 CAPLUS

1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-CN

(trifluoromethyl)phenyl]-N-hydroxy-4-[2,2,2-trifluoro-1-(hydroxyimino)ethyl]- (9CI) (CA INDEX NAME)

### IT 185615-32-1P 185617-32-7P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pyrazole derivs. as insecticides)

RN 185615-32-1 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(2,2,2-trifluoro-1-hydroxyethyl)-(9CI) (CA INDEX NAME)

### RN 185617-32-7 CAPLUS

CN 1H-Pyrazole-3-carboximidamide, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-N-hydroxy-4-(2,2,2-trifluoro-1-hydroxy-1-methylethyl)- (9CI) (CA INDEX NAME)

GI

The title compds. [I; Ar = (un) substituted aromatic hydrocarbyl or heterocycle; R1 = H, halo, NO2, OH, cyano, (un) substituted hydrocarbyl, etc.; R2 = H, halo, NO2, OH, cyano, (un) substituted hydrocarbyl, alkoxy, etc.; X1 = (un) substituted haloalkyl; X2 = H, radical containing C, N, O, S, or P; Y = radical containing O, N, S, or P, (un) substituted aryl, etc.; X2 and Y may together form a hydroxyimino, heterocycle, etc.; R2 and Y may together represent substituted C2-4 alkylene or alkenylene containing O, N, S, or P, etc.] are prepared Insecticides containing I are also claimed. Thus, I (Y1 = Y2 = H) was reacted with (F3CCO)2O in the presence of pyridine to give 38% the title compound II (Y1 = Y2 = F3CCO) (III). III at 100 ppm killed 100% Chilo suppressalis at 3rd-instar larvae.

L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:281619 CAPLUS

DOCUMENT NUMBER:

124:317155

TITLE:

Preparation of halopyrazolecarboxylic acids as

herbicides

INVENTOR(S):

Sato, Kazuo; Kudo, Noriaki; Pponma, Toyokuni; Endo,

Takeshi; Kadotani, Junji; Horibe, Yoshimichi

PATENT ASSIGNEE(S):

SOURCE:

Jpn. Kokai Tokkyo Koho, 26 pp.

CODEN: JKXXAF

Sankyo Co, Japan

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08012654	A2	19960116	JP 1994-144235	19940627
PRIORITY APPLN. INFO.:			JP 1994-144235	19940627
OTHER SOURCE(S):	MARPAT	124:317155		

IT 176232-74-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of halopyrazolecarboxylic acids as herbicides)

RN 176232-74-9 CAPLUS

CN 1H-Pyrazole-3-carboxaldehyde, 4-chloro-1-(2,5-difluorophenyl)-5-phenyl-, oxime (9CI) (CA INDEX NAME)

GI

AB The title compds. I [R = carboxyl, etc.; X = halo; Q1 = Ph, pyridinyl; Q2 = Ph, etc.] are prepared I [X = Cl; Q1 = Q2 = phenyl; R = CO2Me] (m.p. 153 - 155°) (at 10 g/are) gave 91 - 100% control of Echinochloa oryzicola and Scirpus juncoides and caused no damage to rice plants.

L4 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1993:101951 CAPLUS

DOCUMENT NUMBER:

118:101951

TITLE:

Imidazole pesticides

INVENTOR(S):

Willis, Robert John; O'Mahony, Mary Josephine;

Roberts, Bryan Glyn; Marlow, Ian David; Boddy, Ian

Kenneth

PATENT ASSIGNEE(S):

Schering Agrochemicals Ltd., UK

SOURCE:

PCT Int. Appl., 82 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

DOCUMENT T

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 9213451	A1 19920820	WO 1992-GB233	19920210
		JP, KR, PL, RO, RU,	
, , ,		CI, CM, DE, DK, ES,	FR, GA, GB, GN,
	MC, ML, MR, NL,		
AU 9211912	A1 19920907	AU 1992-11912	19920210
PRIORITY APPLN. INFO.:		GB 1991-2834	A 19910211
		GB 1991-2835	A 19910211
		GB 1991-2838	A 19910211
		GB 1991-2841	A 19910211
		GB 1991-2847	A 19910211
		GB 1991-2848	A 19910211
		GB 1991-2857	A 19910211
		GB 1991-14712	A 19910708
		GB 1991-17822	A 19910817

WO 1992-GB233

A 19920210

OTHER SOURCE(S):

MARPAT 118:101951

IT 144910-97-4P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and pesticidal activity of)

RN 144910-97-4 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 2-[5-chloro-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-[(hydroxyimino)methyl]-1H-pyrazol-4-yl]- (9CI) (CA INDEX NAME)

GΙ

alkyl; m = 0, 1, 2; p = 0 or 1 when Z = Z1 or Z2 and is 0 when Z = Z3-Z5] were prepared Thus 0.53 g 3-[(2-amino-1,2-dicyanoethenylimino)methyl]-1-(2,6-dichloro-4-trifluoromethylphenyl)-2,5-dimethylpyrrole was cyclized in the presence of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (0.28 g) in dioxane under reflux for 6 h to give 1-(2,6-dichloro-4trifluoromethylphenyl)-3-(4,5-dicyano-1H-imidazol-2-yl)-2,5dimethylpyrrole. Many examples of I were active insecticides, acaricides, and endoparasiticides in tests (sheep blow fly, blue tick, house fly, cockroach; Trichostrongylus colubriformis).

ANSWER 22 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1990:153721 CAPLUS

DOCUMENT NUMBER:

112:153721

TITLE:

Preparation of pyrazolecarboxylic acid derivatives as

herbicide antidotes for crops

INVENTOR(S):

Sohn, Erich; Mildenberger, Hilmar; Bauer, Klaus;

Bieringer, Hermann

PATENT ASSIGNEE(S):

Hoechst A.-G., Fed. Rep. Ger.

SOURCE:

Eur. Pat. Appl., 57 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				•	
EP 333131	A1	19890920	EP 1989-104500		19890314
EP 333131	B1	19931027			
R: AT, BE, CH,			R, IT, LI, NL, SE		•
DE 3808896			DE 1988-3808896		19880317
AT 96273	E	19931115	AT 1989-104500		19890314
ES 2059596	<b>T</b> 3	19941116	ES 1989-104500		19890314
CN 1035752	Α	19890927	CN 1989-101371		19890315
ZA 8901960	Α	19891025	ZA 1989-1960		19890315
	A5	19901017	DD 1989-326620		19890315
SU 1836012	A3	19930823	SU 1989-4613651		19890315
IL 89620	A1	19941229	IL 1989-89620		19890315
DK 8901286	Α	19890918	DK 1989-1286		19890316
AU 8931373	A1	19890921	AU 1989-31373		19890316
AU 617771	B2	19911205			
BR 8901210	Α	19891031	BR 1989-1210		19890316
JP 01283274	A2	19891114	JP 1989-62325		19890316
CA 1338071	A1	19960220	CA 1989-593977		19890316
HU 49785	A2	19891128	HU 1989-1261		19890317
HU 209734	В	19941028			
AU 9184614	A1	19911114	AU 1991-84614		19910920
AU 634421		19930218			
US 5401700		19950328	US 1992-912659		19920713
US 5945541	A	19990831	US 1994-356659		19941215
PRIORITY APPLN. INFO.:			DE 1988-3808896	Α	19880317
					19890314
•				В1	19890315
				A3	19920713

CASREACT 112:153721; MARPAT 112:153721 OTHER SOURCE(S):

126068-72-2P IT

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as herbicides antidote, for crops)

RN126068-72-2 CAPLUS

1H-Pyrazole-3-carboximidamide, 1-(2,4-dichlorophenyl)-N-hydroxy-5-methyl-CN

(9CI) (CA INDEX NAME)

IT 126068-73-3

RL: BIOL (Biological study)

(safened herbicidal composition, for crops)

RN 126068-73-3 CAPLUS

CN Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester, mixt. with 1-(2,4-dichlorophenyl)-N-hydroxy-5-methyl-1H-pyrazole-3-carboximidamide (9CI) (CA INDEX NAME)

CM 1

CRN 126068-72-2 CMF C11 H10 C12 N4 O

CM 2

CRN 66441-23-4 CMF C18 H16 Cl N O5

GI

$$\begin{array}{c|c}
 & N \\
 & N \\
 & N \\
 & N \\
 & R^2
\end{array}$$

The title compds. I (Y = CH, N; R1 = halo, C1-4-alkyl, -haloalkyl, -alkoxy, etc.; R2 = C1-12 alkyl, C3-7 cycloalkyl; X = CN, CO2R3, COSR3, etc.; R3 = H, alkali or alkaline-earth metal, alkyl, etc.; n = 1-3) are prepared; I can be used in combination with known herbicides, such as phenoxyphenoxy- or heteroaryloxyphenoxycarboxylic esters, chloracetanilides, thiocabamates, and dimedon derivs. I (R1n = 4-Cl, R2 = 5-Me, X = 3-CO2Et) (II) was prepared by reacting Et acetylpyruvate with 4-chlorophenylhydrazine. II (2.5 kg/ha) was tested in combination with fenoxaprop-Et (2 kg/ha) in 800 L aqueous suspension on Triticum aestivum, and resulted in 15% damage to the crops, compared with 80% when using the herbicide alone.

L4 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1972:448115 CAPLUS

DOCUMENT NUMBER:

77:48115

TITLE:

Acylarylnitrosamines. VI. Anomalous reactions with

2,5-dimethylfuran. Formation of 2-benzyl-5-methylfurans and 3-acetyl-1-aryl-4-(arylazo)-5-

methylpyrazoles

AUTHOR (S):

Cadogan, J. I. G.; Mitchell, J. R.; Sharp, J. T.

Dep. Chem., Univ. Edinb., Edinburgh, UK

CORPORATE SOURCE: SOURCE:

Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1972), (11), 1304-10

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE:

Journal English

LANGUAGE:

36845-73-5P 36845-82-6P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 36845-73-5 CAPLUS

CN Ethanone, 1-[1-(4-methoxyphenyl)-4-[(4-methoxyphenyl)azo]-5-methyl-1H-

pyrazol-3-yl]-, oxime (9CI) (CA INDEX NAME)

36845-82-6 CAPLUS RN

Ethanone, 1-(5-methyl-1-phenyl-1H-pyrazol-3-yl)-, oxime (9CI) (CA INDEX CN

RC6H4N(NO)COR1(R = H, or m- or p-CO2Et, MeO-, -Me, R1 = Me; R = H, R1 = Me; R1 =p-ClC6H4) reacted with 2,5-dimethylfuran (I) in excess C6H6 at room temperature;

e.g. PhN(NO)Ac with I in C6H6 gave 27% 2-benzyl-5-methylfuran (II) and 20% 3-acetyl-5-methyl-1-phenyl-4-(phenylazo)-pyrazole (III). II may be formed by  $\pi$ -complexing of the diazonium cation with I, the side-chain protons of which then become sufficiently acidic to be removed by the AcO- counter ion. II may be formed by azo coupling at a vacant 3-position, followed by consecutive ring opening, further coupling, and cyclization under the influence of the diazonium acetate ion pair.

ANSWER 24 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

1967:490758 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 67:90758

Pyrazolo-N-hydroxyuracils from the modified Lossen TITLE:

rearrangement of vicinal pyrazoledicarbohydroxamates

Bauer, Ludwig; Mahajanshetti, Chennabasappa S. AUTHOR (S): Univ. of Illinois Med. Center, Chicago, IL, USA

CORPORATE SOURCE:

Journal of Heterocyclic Chemistry (1967), 4(3), 325-34 SOURCE:

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

17284-61-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(Lossen rearrangement of)

RN17284-61-6 CAPLUS

Pyrazole-3,4-dicarbohydroxamic acid, 1-phenyl-, disodium salt (8CI) (CA

INDEX NAME)

●2 Na

For diagram(s), see printed CA Issue.

AΒ The reaction of 1-phenyl-3,4- and 4,5-pyrazoledicarbohydroxamates, (I) and (II), with benzene- and methanesulfonyl chlorides is reported. Each hydroxamate yielded two isomeric N-phenyl-N-hydroxypyrimidinediones whose structures were established. The N.M.R. spectra of a number of isomeric pyrazole derivs. are discussed. 23 references.

ANSWER 25 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

1963:3269 CAPLUS ACCESSION NUMBER:

58:3269 DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 58:516b-c

Reactions of hydroxymethylene ketones. I. Synthesis of

isoxazoles and pyrazoles from cinnamoylacetaldehyde

and its derivatives

Mina, George Attalah; Rateb, Latif; Soliman, Gabra AUTHOR (S):

Univ. Alexandria, Egypt CORPORATE SOURCE:

Journal of the Chemical Society, Abstracts (1962) SOURCE:

4234-41

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal LANGUAGE: Unavailable OTHER SOURCE(S): CASREACT 58:3269

90946-07-9, Pyrazole-3-carboxaldehyde, 1-phenyl-, oxime

92289-45-7, Ketone, methyl 1-phenylpyrazol-3-yl, oxime

(preparation of) 90946-07-9 CAPLUS RN

Pyrazole-3-carboxaldehyde, 1-phenyl-, oxime (7CI) (CA INDEX NAME) CN

RN92289-45-7 CAPLUS

Ketone, methyl 1-phenylpyrazol-3-yl, oxime (7CI) (CA INDEX NAME) CN

AB The sodium salts of cinnamoylacetaldehyde and its  $\alpha$ -methyl and  $\alpha$ -phenyl derivative have been prepared and used in syntheses of 3- and 5-styrylisoxazoles and 1-phenyl-3- and 5-styrylpyrazoles. The structural formulas of the intermediate monoximes, diisoxazolinylhydroxylamines, and 5-hydroxyaminoisoxazolines are discussed. The isomeric styrylisoxazoles and pyrazoles have been differentiated by oxidation to acidic and ketonic derivs.

=> log y COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	123.95	285.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-18.25	-18.25

STN INTERNATIONAL LOGOFF AT 12:28:17 ON 14 FEB 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1201txs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
                 "Ask CAS" for self-help around the clock
NEWS
NEWS
         SEP 01
                 New pricing for the Save Answers for SciFinder Wizard within
                 STN Express with Discover!
                 KOREAPAT now available on STN
         OCT 28
                 PHAR reloaded with additional data
NEWS
         NOV 30
                 LISA now available on STN
NEWS
         DEC 01
NEWS
         DEC 09
                 12 databases to be removed from STN on December 31, 2004
                 MEDLINE update schedule for December 2004
NEWS
         DEC 15
         DEC 17
                 ELCOM reloaded; updating to resume; current-awareness
NEWS
                 alerts (SDIs) affected
NEWS 10 DEC 17
                 COMPUAB reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
NEWS 11 DEC 17
                 SOLIDSTATE reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
```

NEWS 12 DEC 17 CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected

NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB

NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN

NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED

NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005

NEWS 17 JAN 26 CA/CAPLUS - Expanded patent coverage to include the Russian Agency for Patents and Trademarks (ROSPATENT)

NEWS 18 FEB 10 STN Patent Forums to be held in March 2005

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide (Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 13:16:32 ON 14 FEB 2005

=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 13:16:40 ON 14 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2005 HIGHEST RN 830317-64-1 DICTIONARY FILE UPDATES: 13 FEB 2005 HIGHEST RN 830317-64-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

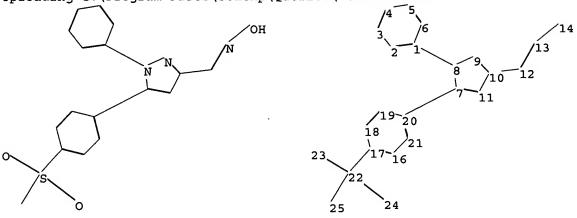
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\106083331.str



chain nodes :

12 13 14 22 23 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 16 17 18 19 20 21

chain bonds :

1-8 7-20 10-12 12-13 13-14 17-22 22-23 22-24 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 16-17 16-21 17-18

18-19 19-20 20-21

exact/norm bonds :

1-8 7-8 8-9 9-10 12-13 13-14 17-22 22-23 22-24 22-25

exact bonds :

7-11 7-20 10-11 10-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

isolated ring systems : containing 1 : 7 : 16 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:CLASS 13:CLASS 14:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS

### L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 13:17:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 1 TO 80

PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L1 L2

=> s l1 ful

FULL SEARCH INITIATED 13:17:07 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -23 TO ITERATE

2 ANSWERS 23 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.01

2 SEA SSS FUL L1 L3

=> file caplus

SINCE FILE TOTAL COST IN U.S. DOLLARS SESSION ENTRY 161.33 161.54 FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:17:16 ON 14 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 14 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 13 Feb 2005 (20050213/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

3 L3

=> d l4 ibib hitstr abs 1-3

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:252948 CAPLUS

DOCUMENT NUMBER: 140:423618

Synthesis and Selective Cyclooxygenase-2 Inhibitory TITLE:

Activity of a Series of Novel, Nitric Oxide

Donor-Containing /Pyrazoles

AUTHOR (S):

Ranatunge Ramani R.; Augustyniak, Michael; Bandarage, Upul K.; Earl, Richard A.; Ellis, James L.; Garvey, David S.; Janero, David R.; Letts, L. Gordon; Martino, Allison M.; Murty, Madhavi G.; Richardson, Stewart K.; Schroeder, Joseph D.; Shumway, Matthew J.; Tam, S.

William; Trocha, A. Mark; Young, Delano V.

NitroMed Inc., Bedford, MA, 01730, USA CORPORATE SOURCE:

Journal of Medicinal Chemistry (2004), 47(9), SOURCE:

2180-2193

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: DOCUMENT TYPE: American Chemical Society

Journal English

LANGUAGE:

TT

CN

640727-97-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and selective cyclooxygenase-2 inhibitory activity of nitric oxide donor-containing pyrazoles)

640727-97-5 CAPLUS RN

> Benzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} CN \\ O \\ S-Me \\ O \\ O \\ N \end{array}$$

GI

Ι

The synthesis of a series of novel pyrazoles containing a nitrate (ONO2) AB moiety as a nitric oxide (NO)-donor functionality is reported. Their COX-1 and COX-2 inhibitory activities in human whole blood are profiled. The data demonstrate that pyrazole ring substituents play an important role in COX-2 selective inhibition, such that a cycloalkylpyrazole (I, X = CH2) was found to be a potent and selective COX-2 inhibitor. Other modifications at the 3 position of the central pyrazole ring [I, X = (CH2)3, C(:NOH)(CH2)3, (Z)-CH:CHCH2CH2] enhanced COX-2 inhibitory potency. Among the pyrazoles synthesized, the oxime [I, X = C(:NOH)(CH2)3] was identified as the most potent COX-2 selective inhibitor. Accordingly, this compound was profiled pharmacol. in the rat after oral administration

and shown to possess potent antiinflammatory activity in the carrageenan-induced air-pouch model and less gastric toxicity than a standard COX-2 inhibitor when administered with background aspirin treatment. The enhanced gastric tolerance of an NO-donor COX-2 selective inhibitor has the potential to augment the clin. profile of this drug class.

REFERENCE COUNT: THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS 52 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

2004:20441 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 140:77147

TITLE: Preparation of optionally nitrosated and/or

nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compositions and methods of use

Garvey, David S.; Ranatunge, Ramani R.; Richardson, INVENTOR(S):

Stewart K.

PATENT ASSIGNEE(S): Nitromed, Inc., USA PCT Int. Appl., 166 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

```
APPLICATION NO.
    PATENT NO.
                      KIND
                               DATE
                                                                 DATE
                               -----
                        ----
                                          _____
                                                                 _____
                                         WO 2003-US20421
                        A2
                               20040108
                                                                 20030630
    WO 2004002420
                        A3
    WO 2004002420
                               20040701
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                           US 2002-392044P
PRIORITY APPLN. INFO.:
                                                             P 20020628
                        MARPAT 140:77147
OTHER SOURCE(S):
    640727-83-9P, 1-[3-[1-(Hydroxyimino)-4-(nitrooxy)butyl]-1-
    phenylpyrazol-5-yl]-4-(methylsulfonyl)benzene 640727-97-5P,
    4-[3-[1-(Hydroxyimino)-4-(nitrooxy)butyl]-5-[4-
     (methylsulfonyl)phenyl]pyrazol-1-yl]benzenecarbonitrile
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of optionally nitrosated and/or nitrosylated
        oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compns.
       and methods of use)
    640727-83-9 CAPLUS
RN
CN
```

1-Butanone, 1-[5-[4-(methylsulfonyl)phenyl]-1-phenyl-1H-pyrazol-3-yl]-4-(nitrooxy) -, oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ &$$

RN 640727-97-5 CAPLUS
CN Benzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

$$O_2N-O-(CH_2)_3-C$$
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 

GΙ

$$\begin{array}{c}
 & \text{R1} \\
 & \text{R1} \\
 & \text{R2} \\
\end{array}$$

$$\begin{array}{c}
 & \text{C} \\
 & \text{Z1} \\
 & \text{Y1} \\
 & \text{R2} \\
\end{array}$$

The invention describes novel cyclooxygenase 2 (COX-2) selective AΒ inhibitors having at least one oxime group or hydrazone group optionally nitrosated and/or nitrosylated (one class shown as I; variables defined below; e.g. II; 15 other classes of compds. are also described in the 1st claim) and novel compns. and kits comprising at least one I and optionally, at least one compound that donates, transfers or releases nitric oxide, stimulates endogenous synthesis of nitric oxide, elevates endogenous levels of endothelium-derived relaxing factor or is a substrate for nitric oxide synthase, and/or at least one therapeutic agent. The invention also provides methods for treating inflammation, pain and fever; for treating and/or improving the gastrointestinal properties of COX-2 selective inhibitors; for facilitating wound healing; for treating and/or preventing renal and/or respiratory toxicity; for treating and/or preventing other disorders resulting from elevated levels of cyclooxygenase-2; and for improving the cardiovascular profile of COX-2 selective inhibitors. Six examples of I were tested for inhibition of COX-1 and COX-2; e.g. 1-[1-cyclohexyl-3-[1-(hydroxyimino)-4-(nitrooxy)butyl]pyrazol-4-yl]-4-(methylsulfonyl)benzene inhibited COX-1 10 % at 100  $\mu M$  and COX-2 100 % at 10  $\mu M$ . Although the methods of preparation are not claimed, 6 example prepns. are included. For example, II was prepared in 7 steps (79, 68, 84, 79, 51, 84 and 48 % yields, resp.) starting from di-Me oxalate, NaOMe and 4'-(methylthio)acetophenone in toluene and involving intermediates Me (2Z)-2-hydroxy-4-(4methylthiophenyl) -4-oxobut-2-enoate, Me 5-(4-methylthiophenyl) -1phenylpyrazole-3-carboxylate, N-methoxy-N-methyl-5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxamide, 1-[5-(4-methylthiophenyl)-1-phenylpyrazol-3yl]-4-(1,1,2,2-tetramethyl-1-silapropoxy)butan-1-one, 4-hydroxy-1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]butan-1-one, and 1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]-4-(nitrooxy)butan-1one. For I: when side b is a double bond, and sides a and c are single bonds, -X1-Y1-Z1- is: -CR4(R5)CR5(R5')CR4(R5)-, -C(O)CR4(R4')CR5(R5')-, -CR4(R4')CR5(R5')C(0)-, -[CR5(R5')]kOC(0)-, etc.; when sides a and c are double bonds and side b is a single bond, -X1-Y1-Z1- is: :CR40CR5:,

II

:CR4NR3CR5:, :NSCR4:, :CR4SN:, etc. R1 is S(0)2Me, S(0)2NR8(D1), S(O) 2N(D1)C(O)CF3, S(O)(NH)NH(D1), S(O)(NH)N(D1)C(O)CF3, P(O)MeNH(D1), P(O)Me2, C(S)NH(D1), S(O)(NH)Me, P(O)MeOD1, or P(O)MeNH(D1); R1' is H, halo, Me, or CH2OH. R2 is lower alkyl, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, mono, di- or trisubstituted heteroaryl (wherein the heteroaryl is a monocyclic aromatic ring of 5 atoms, said ring having one heteroatom which is S, O, or N, and, optionally, 1-3 addnl. N atoms; or the heteroaryl is a monocyclic ring of 6 atoms, said ring having one heteroatom which is N, and, optionally, 1-4 addnl. N atoms), benzoheteroaryl, NR10R11, SR11, OR11, R11, alkenyl, alkynyl, unsubstituted, mono, di, tri- or tetrasubstituted cycloalkenyl, mono, di, tri- or tetrasubstituted heterocycloalkyl group of 5-7 members, or a benzoheterocycle, wherein said heterocycloalkyl or benzoheterocycle contains 1 or 2 heteroatoms selected from O, S, or N and, optionally, contains a carbonyl group or a sulfonyl group, styryl, mono or disubstituted styryl, phenylacetylene, mono- or disubstituted phenylacetylene, fluoroalkenyl, mono- or disubstituted bicyclic heteroaryl of 8-10 members, containing 2-5 heteroatoms (wherein at least one heteroatom resides on each ring of said bicyclic heteroaryl, said heteroatoms are each independently O, S and N), K, aryl, arylalkyl, cycloalkylalkyl, -C(O)R11, hydrogen, arylalkenyl, arylalkoxy, alkoxy, aryloxy, cycloalkoxy, arylthio, alkylthio, arylalkylthio, or cycloalkylthio. R3 is hydrogen, haloalkyl (preferably CF3), CN, lower alkyl, [C(Re)(Rf)]p-U-V, K, (un) substituted lower alkyl-Q, lower alkyl-O-lower alkyl-Q, etc., Q, alkylcarbonyl, arylcarbonyl, alkylarylcarbonyl, arylalkylcarbonyl, carboxylic ester, carboxamido, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, alkenyl, alkynyl, arylalkyl, lower alkyl-OD1, alkoxyalkyl, aminoalkyl, lower alkyl-CO2R10, lower alkyl-C(O)NR10(R10'), heterocyclic alkyl, or heterocyclic ring-C(O)-; with the proviso that one oxime or hydrazone group must be present; addnl. details are given in the claims.

```
ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
```

ACCESSION NUMBER:

2004:20345 CAPLUS

DOCUMENT NUMBER: TITLE:

140:77144 Preparation of optionally nitrosated and/or

nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compositions and methods of use

INVENTOR (S):

Ranatunge, Ramana R.; Garvey, David S.; Richardson,

Stewart K.

PATENT ASSIGNEE(S):

Nitromed, Inc., USA

SOURCE:

U.S. Pat. Appl. Publ., 74 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004006133	A1	20040108	US 2003-608333	20030630
PRIORITY APPLN. INFO.:			US 2002-392044P P	20020628

OTHER SOURCE(S): MARPAT 140:77144 640727-83-9P 640727-97-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of optionally nitrosated and/or nitrosylated oxime and/or hydrazone cyclooxygenase-2 selective inhibitors, compns. and methods of use)

640727-83-9 CAPLUS RN

CN 1-Butanone, 1-[5-[4-(methylsulfonyl)phenyl]-1-phenyl-1H-pyrazol-3-yl]-4-(nitrooxy)-, oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ &$$

RN 640727-97-5 CAPLUS
CN Benzonitrile, 4-[3-[1-(hydroxyimino)-4-(nitrooxy)butyl]-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

$$O_2N-O-(CH_2)_3-C$$
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 
 $O_2N-O-(CH_2)_3-C$ 

GI

AB The invention describes novel cyclooxygenase 2 (COX-2) selective inhibitors having at least one oxime group or hydrazone group optionally nitrosated and/or nitrosylated (one class shown as I; variables defined below; e.g. II; 15 other classes of compds. are also described in the 1st claim) and novel compns. and kits comprising at least one I and optionally, at least one compound that donates, transfers or releases nitric oxide, stimulates endogenous synthesis of nitric oxide, elevates endogenous levels of endothelium-derived relaxing factor or is a substrate for nitric oxide synthase, and/or at least one therapeutic agent. The invention also provides methods for treating inflammation, pain and fever; for treating and/or improving the gastrointestinal properties of COX-2 selective inhibitors; for facilitating wound healing; for treating and/or preventing renal and/or respiratory toxicity; for treating and/or preventing other disorders resulting from elevated levels of cyclooxygenase-2; and for improving the cardiovascular profile of COX-2 selective inhibitors. Six examples of I were tested for inhibition of COX-1 and COX-2; e.g. 1-[1-cyclohexyl-3-[1-(hydroxyimino)-4-(nitrooxy)butyl]pyrazol-4-yl]-4-(methylsulfonyl)benzene inhibited COX-1 10 % at 100  $\mu$ M and COX-2 100 % at 10  $\mu$ M. Although the methods of preparation are not claimed, 6 example prepns. are included. For example, II was prepared in 7 steps (79, 68, 84, 79, 51, 84 and 48 % yields, resp.) starting from di-Me oxalate, NaOMe and 4'-(methylthio)acetophenone in toluene and involving intermediates Me (2Z)-2-hydroxy-4-(4methylthiophenyl)-4-oxobut-2-enoate, Me 5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxylate, N-methoxy-N-methyl-5-(4-methylthiophenyl)-1phenylpyrazole-3-carboxamide, 1-[5-(4-methylthiophenyl)-1-phenylpyrazol-3y1]-4-(1,1,2,2-tetramethyl-1-silapropoxy) butan-1-one, 4-hydroxy-1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]butan-1-one, and 1-[5-[4-(methylsulfonyl)phenyl]-1-phenylpyrazol-3-yl]-4-(nitrooxy)butan-1one. For I: when side b is a double bond, and sides a and c are single bonds, -X1-Y1-Z1- is: -CR4(R5)CR5(R5')CR4(R5)-, -C(0)CR4(R4')CR5(R5')-, -CR4(R4')CR5(R5')C(O)-, -[CR5(R5')]kOC(O)-, etc.; when sides a and c are double bonds and side b is a single bond, -X1-Y1-Z1- is: :CR40CR5:,

II

:CR4NR3CR5:, :NSCR4:, :CR4SN:, etc. R1 is S(0)2Me, S(0)2NR8(D1), S(0) 2N(D1)C(0)CF3, S(0)(NH)NH(D1), S(0)(NH)N(D1)C(0)CF3, P(0)MeNH(D1), P(O)Me2, C(S)NH(D1), S(O)(NH)Me, P(O)MeOD1, or P(O)MeNH(D1); R1' is H, halo, Me, or CH2OH. R2 is lower alkyl, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, mono, di- or trisubstituted heteroaryl (wherein the heteroaryl is a monocyclic aromatic ring of 5 atoms, said ring having one heteroatom which is S, O, or N, and, optionally, 1-3 addnl. N atoms; or the heteroaryl is a monocyclic ring of 6 atoms, said ring having one heteroatom which is N, and, optionally, 1-4 addnl. N atoms), benzoheteroaryl, NR10R11, SR11, OR11, R11, alkenyl, alkynyl, unsubstituted, mono, di, tri- or tetrasubstituted cycloalkenyl, mono, di, tri- or tetrasubstituted heterocycloalkyl group of 5-7 members, or a benzoheterocycle, wherein said heterocycloalkyl or benzoheterocycle contains 1 or 2 heteroatoms selected from O, S, or N and, optionally, contains a carbonyl group or a sulfonyl group, styryl, mono or disubstituted styryl, phenylacetylene, mono- or disubstituted phenylacetylene, fluoroalkenyl, mono- or disubstituted bicyclic heteroaryl of 8-10 members, containing 2-5 heteroatoms (wherein at least one heteroatom resides on each ring of said bicyclic heteroaryl, said heteroatoms are each independently O, S and N), K, aryl, arylalkyl, cycloalkylalkyl, -C(O)R11, hydrogen, arylalkenyl, arylalkoxy, alkoxy, aryloxy, cycloalkoxy, arylthio, alkylthio, arylalkylthio, or cycloalkylthio. R3 is hydrogen, haloalkyl (preferably CF3), CN, lower alkyl, [C(Re)(Rf)]p-U-V, K, (un) substituted lower alkyl-Q, lower alkyl-O-lower alkyl-Q, etc., Q, alkylcarbonyl, arylcarbonyl, alkylarylcarbonyl, arylalkylcarbonyl, carboxylic ester, carboxamido, cycloalkyl, mono, di- or trisubstituted Ph or naphthyl, alkenyl, alkynyl, arylalkyl, lower alkyl-OD1, alkoxyalkyl, aminoalkyl, lower alkyl-CO2R10, lower alkyl-C(0)NR10(R10'), heterocyclic alkyl, or heterocyclic ring-C(0)-; with the proviso that one oxime or hydrazone group must be present; addnl. details are given in the claims.

=> log y COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.27	176.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.19

STN INTERNATIONAL LOGOFF AT 13:17:38 ON 14 FEB 2005